

JANUARY 1999

ISSN 0301-0104

Chemical Physics

**A journal devoted to experimental and theoretical research
involving problems of both a chemical and a physical nature**

MASTER INDEX

VOLUMES 231-240

MAY 1998 – JANUARY 1999

Editors

ROBIN M. HOCHSTRASSER

G. LUDWIG HOFACKER

H. PETER TROMMSDORFF

NORTH-HOLLAND

Chemical Physics

A journal devoted to experimental and theoretical research involving problems of both a chemical and a physical nature

EDITORS

ROBIN M. HOCHSTRASSER

Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323, USA

Fax: 1-215-8980590; E-mail: hochstra@chem.upenn.edu

G. LUDWIG HOFACKER

Lehrstuhl für Theoretische Chemie, Technische Universität München, Lichtenbergstrasse 4, 85747 Garching, Germany

Fax: 49-89-28913622; E-mail: hofacker@theochem.tu-muenchen.de

H. PETER TROMMSDORFF

Laboratoire de Spectrométrie Physique, Université Joseph Fourier de Grenoble - CNRS, B.P. 87, 38402 Saint-Martin-d'Hères Cedex, France

Fax: 33-476-514335; E-mail: chemphys@ujf-grenoble.fr

ASSOCIATE EDITOR

DAVID CHANDLER

Department of Chemistry, University of California Berkeley, Berkeley, CA 94720, USA

Fax: 1-510-6428369; E-mail: chandler@cchem.berkeley.edu

ADVISORY EDITORIAL BOARD

Australia

D.J. EVANS, Canberra

N.S. HUSH, Sydney

R.O. WATTS, Mulgrave

Canada

R.J.D. MILLER, Toronto

Denmark

G.D. BILLING, Copenhagen

France

S. LEACH, Meudon

D. MARKOVITSI, Gif-sur-Yvette

J.L. MARTIN, Palaiseau

M. ORRIT, Talence

Germany

H. BÄSSLER, Marburg

B. DICK, Regensburg

S.F. FISCHER, Garching

H. GRABERT, Freiburg

D. HAARER, Bayreuth

P. HÄNGGI, Augsburg

W. LORENZ, Leipzig

D. MENZEL, Garching

M. PARRINELLO, Stuttgart

E.W. SCHLAG, Garching

W. ZINTH, Munich

Hungary

P. ORMOS, Szeged

Israel

R.B. GERBER, Jerusalem

J. JORTNER, Tel Aviv

R.D. LEVINE, Jerusalem

E. POLLAK, Rehovot

Italy

G. CICCOTTI, Rome

Japan

H. HAMAGUCHI, Tokyo

M. ITO, Okazaki

T. KITAGAWA, Okazaki

T. KOBAYASHI, Tokyo

K. YOSHIHARA, Ishikawa

The Netherlands

D. FRENKEL, Amsterdam

Russian Federation

V.S. LETOKHOV, Moscow

Sweden

R. RIGLER, Stockholm

Switzerland

H. FISCHER, Zurich

S. LEUTWYLER, Bern

Taiwan

Y.T. LEE, Taipei

United Kingdom

A.D. BUCKINGHAM, Cambridge

D.A. KING, Cambridge

P.A. MADDEN, Oxford

J.P. SIMONS, Oxford

USA

A.C. ALBRECHT, Ithaca, NY

P. ALIVISATOS, Berkeley, CA

V.A. APKARIAN, Irvine, CA

P.F. BARBARA, Austin, TX

R. BERSOHN, New York, NY

S.G. BOXER, Stanford, CA

S.T. CEYER, Cambridge, MA

K.A. DILL, San Francisco, CA

W.A. EATON, Bethesda, MD

M.D. FAYER, Stanford, CA

G.R. FLEMING, Berkeley, CA

G. FLYNN, New York, NY

R.A. FRIESNER, New York, NY

M. KLEIN, Philadelphia, PA

USA (continued)

W.C. LINEBERGER, Boulder, CO

D.S. McCLURE, Princeton, NJ

D.M. NEUMARK, Berkeley, CA

M.D. NEWTON, Upton, NY

C.S. PARMENTER,

Bloomington, IN

M.A. RATNER, Evanston, IL

G.W. ROBINSON, Lubbock, TX

G.J. SMALL, Ames, IA

J.C. TULLY, New Haven, CT

J.D. WEEKS, College Park, MD

K.B. WHALEY, Berkeley, CA

P.G. WOLYNES, Urbana, IL

R.N. ZARE, Stanford, CA

A.H. ZEWAIL, Pasadena, CA

AIMS AND SCOPE

Chemical Physics publishes experimental and theoretical papers on all aspects of chemical physics. Experimental papers are brought into relation with theory and theoretical papers demonstrate their relation to present or future experiments. More specifically, subject matter in the fields of spectroscopy and molecular structure, interacting systems, relaxation phenomena, fundamental problems in molecular reactivity, molecular quantum theory and statistical mechanics constitute the main areas of interest for this journal. In addition to regular issues, *Chemical Physics* publishes thematic issues containing invited articles by specialists in the relevant field.

Chemical Physics

EDITORS

ROBIN M. HOCHSTRASSER

Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323, USA

Fax: 1-215-8980590; E-mail: hochstra@a.chem.upenn.edu

G. LUDWIG HOFACKER

Lehrstuhl für Theoretische Chemie, Technische Universität München, Lichtenbergstrasse 4, 85747 Garching, Germany

Fax: 49-89-28913622; E-mail: hofacker@theochem.tu-muenchen.de

H. PETER TROMMSDORFF

Laboratoire de Spectrométrie Physique, Université Joseph Fourier de Grenoble - CNRS, B.P. 87, 38402 Saint-Martin-d'Hères Cedex, France

Fax: 33-476-514335; E-mail: chemphys@ujf-grenoble.fr

ASSOCIATE EDITOR

DAVID CHANDLER

Department of Chemistry, University of California Berkeley, Berkeley, CA 94720, USA

Fax: 1-510-6428369; E-mail: chandler@cchem.berkeley.edu

ADVISORY EDITORIAL BOARD

Australia

D.J. EVANS, Canberra

N.S. HUSH, Sydney

R.O. WATTS, Mulgrave

Canada

R.J.D. MILLER, Toronto

Denmark

G.D. BILLING, Copenhagen

France

S. LEACH, Meudon

D. MARKOVITSI, Gif-sur-Yvette

J.L. MARTIN, Palaiseau

M. ORRIT, Talence

Germany

H. BÄSSLER, Marburg

B. DICK, Regensburg

S.F. FISCHER, Garching

H. GRABERT, Freiburg

D. HAARER, Bayreuth

P. HÄNGGI, Augsburg

W. LORENZ, Leipzig

D. MENZEL, Garching

M. PARRINELLO, Stuttgart

E.W. SCHLAG, Garching

W. ZINTH, Munich

Hungary

P. ORMOS, Szeged

Israel

R.B. GERBER, Jerusalem

J. JORTNER, Tel Aviv

R.D. LEVINE, Jerusalem

E. POLLAK, Rehovot

Italy

G. CICCOTTI, Rome

Japan

H. HAMAGUCHI, Tokyo

M. ITO, Okazaki

T. KITAGAWA, Okazaki

T. KOBAYASHI, Tokyo

K. YOSHIHARA, Ishikawa

The Netherlands

D. FRENKEL, Amsterdam

Russian Federation

V.S. LETOKHOV, Moscow

Sweden

R. RIGLER, Stockholm

Switzerland

H. FISCHER, Zurich

S. LEUTWYLER, Bern

Taiwan

Y.T. LEE, Taipei

United Kingdom

A.D. BUCKINGHAM, Cambridge

D.A. KING, Cambridge

P.A. MADDEN, Oxford

J.P. SIMONS, Oxford

USA

A.C. ALBRECHT, Ithaca, NY

P. ALIVISATOS, Berkeley, CA

V.A. APKARIAN, Irvine, CA

P.F. BARBARA, Austin, TX

R. BERSOHN, New York, NY

S.G. BOXER, Stanford, CA

S.T. CEYER, Cambridge, MA

K.A. DILL, San Francisco, CA

W.A. EATON, Bethesda, MD

M.D. FAYER, Stanford, CA

G.R. FLEMING, Berkeley, CA

G. FLYNN, New York, NY

R.A. FRIESNER, New York, NY

M. KLEIN, Philadelphia, PA

USA (continued)

W.C. LINEBERGER, Boulder, CO

D.S. McCLURE, Princeton, NJ

D.M. NEUMARK, Berkeley, CA

M.D. NEWTON, Upton, NY

C.S. PARMENTER, Bloomington, IN

M.A. RATNER, Evanston, IL

G.W. ROBINSON, Lubbock, TX

G.J. SMALL, Ames, IA

J.C. TULLY, New Haven, CT

J.D. WEEKS, College Park, MD

K.B. WHALEY, Berkeley, CA

P.G. WOLYNES, Urbana, IL

R.N. ZARE, Stanford, CA

A.H. ZEWAHL, Pasadena, CA

Abstracted/indexed in: Chemical Abstracts, ERDA Abstracts, ISI Current Contents, Inspec Abstracts, Nuclear Engineering Abstracts, Physics Abstracts, Physikalische Berichte/Physics Briefs.

Chemical Physics

Editors

ROBIN M. HOCHSTRASSER, Philadelphia

G. LUDWIG HOFACKER, Munich

H. PETER TROMMSDORFF, Grenoble

Associate Editors

DAVID CHANDLER, Berkeley

MASTER INDEX

VOLUMES 231-240

MAY 1998 - JANUARY 1999



ELSEVIER

Amsterdam - Lausanne - New York - Oxford - Shannon - Tokyo

© 1999, Elsevier Science B.V. All rights reserved

This journal and the individual contributions contained in it are protected under copyright of Elsevier Science B.V., and the following terms and conditions apply to their use:

Photocopying

Single photocopies of single articles may be made for personal use as allowed by national copyright laws. Permission of the Publisher and payment of a fee is required for all other photocopying, including multiple or systematic copying, copying for advertising or promotional purposes, resale, and all forms of document delivery. Special rates are available for educational institutions that wish to make photocopies for non-profit educational classroom use.

Permissions may be sought directly from Elsevier Science Rights & Permissions Department, PO Box 800, Oxford OX5 1DX, UK; phone: (+44) 1865 843830, fax: (+44) 1865 853333, e-mail: permissions@elsevier.co.uk. You may also contact Rights & Permissions directly through Elsevier's home page (<http://www.elsevier.nl>), selecting first 'Customer Support', then 'General Information', then 'Permissions Query Form'.

In the USA, users may clear permissions and make payments through the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923, USA; phone: (+1) (978) 7508400, fax: (+1) (978) 7504744, and in the UK through the Copyright Licensing Agency Rapid Clearance Service (CLARCS), 90 Tottenham Court Road, London W1P 0LP, UK; phone: (+44) 171 436 5931; fax: (+44) 171 436 3986. Other countries may have a local reprographic rights agency for payments.

Derivative Works

Subscribers may reproduce tables of contents or prepare lists of articles including abstracts for internal circulation within their institutions. Permission of the Publisher is required for resale or distribution outside the institution.

Permission of the Publisher is required for all other derivative works, including compilations and translations.

Electronic Storage or Usage

Permission of the publisher is required to store or use electronically any material contained in this journal, including any article or part of an article. Contact the Publisher at the address indicated.

Except as outlined above, no part of this publication may be reproduced, stored in a retrieval system or transmitted in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, without prior written permission of the Publisher.

Address permissions requests to: Elsevier Science Rights & Permissions Department, at the mail, fax and e-mail addresses noted above.

Notice

No responsibility is assumed by the Publisher for any injury and/or damage to persons or property as a matter of products liability, negligence or otherwise, or from any use or operation of any methods, products, instructions or ideas contained in the material herein. Because of rapid advances in the medical sciences, in particular, independent verification of diagnoses and drug dosages should be made.

Although all advertising material is expected to conform to ethical (medical) standards, inclusion in this publication does not constitute a guarantee or endorsement of the quality or value of such product or of the claims made of it by its manufacturer.

Elsevier Science B.V.

Tel: (+31-20)4852-800 Fax: (+31-20)4852-775 E-mail: e.hovens@elsevier.nl

Postal Address

Chemical Physics
Elsevier Science B.V.
P.O. Box 2759
1000 CT Amsterdam
The Netherlands

Courier Service Address

Chemical Physics
Elsevier Science B.V.
Sara Burgerhartstraat 25
1055 KV Amsterdam
The Netherlands

∞ The paper used in this publication meets the requirements of ANSI/NISO Z39.48-1992 (Permanence of Paper)

Printed in the Netherlands.

Contents

Author index to volumes 231-240	1	Photon counting and phase fluorimetry	53
Subject index to volumes 231-240	33	Photoelectron and Auger spectroscopy	53
METHODS AND CONSTRUCTS	33	Multiphoton ionization	54
<i>Theoretical</i>	33	X-ray spectroscopy	55
Computational methods for electronic structure	33	Electron impact spectroscopy	55
CI and valence bond approach	35	Laser induced fluorescence	55
perturbative and many body approaches	36	Ultrafast measurements	56
density functional theory	36	Nonlinear optics and spectroscopy	57
Semiempirical methods	37	Synchrotron spectroscopies	57
Algebraic approaches	38	Coherent optical spectroscopy	58
Relativistic electronic structure theory	38	Atomic and molecular beam techniques	58
Wavefunctions for highly excited and unbound states	38	Mass spectroscopy	59
Spin states and magnetic interactions	39	Radiolysis	60
Molecular response to external fields (incl. optical susceptibilities, dichroism, hyperpolarizabilities)	39	X-ray, electron and neutron diffraction	60
Radiative (incl. relativistic) effects on molecules and molecular processes	40	Neutron scattering (inelastic and quasielastic)	60
Scattering of waves and particles	41	Light scattering	60
Collisional and reactive molecular dynamics with non-frictional forces	41	OBJECTS	60
Reactive molecular dynamics including dissipative processes	42	<i>Bulk systems</i>	60
Intramolecular dynamics	43	Gases	60
Molecular dynamics of many particle systems and condensed phases	43	Supersonic beams	63
Quasiparticle dynamics (incl. excitons, polarons)	44	Liquids neat	63
Migration and interaction on grids and lattices	44	Liquid mixtures and solutions	64
Statistical computational methods (incl. Monte Carlo)	45	Crystals	65
Dynamics of structures, lattices and macromolecular conformations	45	neat	66
Fluctuations and random processes	45	mixed	66
Non-equilibrium statistical mechanics	46	Glasses	66
Non-equilibrium thermodynamic and hydrodynamic theories	46	Complex fluids	66
Equilibrium statistical mechanics and thermodynamics	47	liquid crystals	67
Extremum methods for ensembles (energy, entropy, free energy)	47	colloidal suspensions	67
Theory of critical behaviour	47	Polymers	67
Time and space correlation functions	47	Semiconductors	67
<i>Experiment</i>	47	Metals and alloys	67
Magnetic resonances	47	Thin films	67
Molecular spectroscopy	48	Surfaces	68
microwave	49	Low-dimensional materials	68
infrared	50	Dielectrics	68
Raman	51	Plasmas	68
UV	51	Biological systems	69
visible	53	<i>Microscopic and mesoscopic systems</i>	69
		Single atoms, molecules and assemblies (incl. biological)	69
		Molecules (neutral and ionic)	70
		diatomic	71

small polyatomics	72	Photochemistry	93
aromatics	74	Intramolecular dynamics	94
other large	75	radiationless transitions	95
polymeric and biological	75	vibrational energy redistribution (incl. vibrational dissociation)	95
Molecular aggregates	76	Luminescence spectra, yields and lifetimes	95
dimers	76	Coherence loss processes	96
van der Waals molecules	77	Nonlinear responses (incl. optical)	96
clusters	78	Multiphoton phenomena	96
complexes	79	Reactions (incl. dissociation)	97
Free radicals (incl. hydronium and muonium)	80	isolated molecules	98
Quasiparticles (incl. excitons)	81	collisional	98
Defects and impurities	81	condensed phase	99
Ions and charge carriers	81	Tunneling	99
Supramolecular assemblies (incl. nanoparticles and nanostructures)	81	Electron transfer	100
Liquid-liquid and liquid-solid interfaces	81	Proton and hydrogen atom transfer	101
Biological assemblies, cells and organelles	81	Positron annihilation	102
Proteins	82	Ionization (incl. Rydberg states)	102
Nucleic acids	82	Molecular motion (incl. diffusive)	102
Membranes	82	Isotopic effects	103
<i>PHENOMENA</i>	82	Fluctuations and noise	103
Molecular structure	82	Surface chemical physics	103
Vibrations and rotations of molecules	84	surface scattering	104
Electronic structures and states	86	adsorption	104
Electric and magnetic properties	88	desorption	104
Spin splittings	88	surface excitations	104
Optical activity	88	adsorbate structure	104
Molecular interactions	89	surface reactions	104
Spectral bandshapes and intensities	90	catalysis	104
Coupling of electronic and nuclear motion	91	Electronic process in gases	104
Energy transfer processes	91	Thermodynamic and transport properties	105
Molecular photophysical processes	92	Structure of solids, liquids and glasses	105
		Critical behavior and phase transitions	105
		Molecular self-assembly and -organization	106

Author index to volumes 231–240

- Abrahão Junior, O., see Alemán, C. 233 (1998) 85
- Achatz, U., see Berg, C. 239 (1998) 379
- Adamowicz, L., see Desfrancois, C. 239 (1998) 475
- Adhikari, S. and G.D. Billing, Semiclassical reactive scattering: the Hermite correction method in hyperspherical coordinates 238 (1998) 69
- Agranovich, V.M., see Kiselev, S.A. 238 (1998) 365
- Ågren, H., see Plashkevych, O. 232 (1998) 49
- Ågren, H., see Engström, M. 237 (1998) 149
- Ågren, H., see Magnuson, M. 237 (1998) 295
- Agui, A., see Magnuson, M. 237 (1998) 295
- Ahern, M.M., see Belikov, A.E. 234 (1998) 195
- Aiuchi, K., see Tsuji, K. 231 (1998) 279
- Albrecht, A.C., see Ulness, D.J. 240 (1999) 109
- Alemán, C. and S.E. Galembeck, Solvation of chromone using combined Discrete/SCRF models 232 (1998) 151
- Alemán, C., H.M. Ishiki, E.A. Armelin, O. Abrahão Junior and S.E. Galembeck, Free energies of solvation for peptides and polypeptides using SCRF methods 233 (1998) 85
- Alexander, M.H., X. Li, R. Liyanage and R.J. Gordon, Spin-orbit branching in the predissociation of the $C^1\Pi$ state of HCl and DCl: a manifestation of quantum interference 231 (1998) 331
- Alikhani, M.E., see Krim, L. 237 (1998) 265
- Alonso, J.L., see Melandri, S. 239 (1998) 229
- Alvira, E., J.I. García and J.A. Mayoral, Molecular modelling study for chiral separation of equol enantiomers by β -cyclodextrin 240 (1999) 101
- Amar, F.G., see Parneix, P. 239 (1998) 121
- Amat-Guerri, F., see López Arbeloa, F. 236 (1998) 331
- Amorim, J., see Loureiro, J. 232 (1998) 141
- Anderson, D.T., M. Schuder and D.J. Nesbitt, Large-amplitude motion in highly quantum clusters: high-resolution infrared absorption studies of jet-cooled H_2 -HCl and H_2 -DCI 239 (1998) 253
- Anderson, H.L., see Qureshi, F.M. 231 (1998) 87
- Andruniow, T. and M. Pawlikowski, Franck-Condon effects in low-energy states of $C_{10}H_8^+$ radical. Ab initio MCSCF study of absorption and resonance Raman spectra 236 (1998) 25
- Andruniow, T. and M. Pawlikowski, Vibronic coupling effects in the low-energy 1^2B_{1g} and 2^2B_{1g} states of the $C_{10}H_8^+$ radical 236 (1998) 35
- Ankerhold, J., see Pechukas, P. 235 (1998) 5
- Apkarian, V.A., see Grigorenko, B.L. 232 (1998) 321
- Apkarian, V.A., see Zadoyan, R. 233 (1998) 353

- Arai, M., see Ikushima, Y. 238 (1998) 455
Armelin, E.A., see Alemán, C. 233 (1998) 85
Arrivo, S.M., see Kleiman, V.D. 233 (1998) 207
Asada, T., see Watanabe, H. 237 (1998) 81
Ashfold, M.N.R., see Langford, S.R. 231 (1998) 245
Atkinson, D.B., see Fahr, A. 236 (1998) 43
Avaldi, L., see Feng, R. 240 (1999) 371
Ayotte, P., G.H. Weddle, J. Kim and M.A. Johnson, Mass-selected "matrix isolation" infrared spectroscopy of the $\text{I}^- \cdot (\text{H}_2\text{O})_2$ complex: making and breaking the inter-water hydrogen-bond 239 (1998) 485
Azriel, V.M., L.Yu. Rusin, M.B. Sevryuk and J.P. Toennies, Effect of the angular dependence of the barrier height on the features of the $\text{F} + \text{H}_2$ reaction 232 (1998) 307
- Bacchus-Montabonel, M.C., Charge transfer recombination of Si^{2+} ions from atomic hydrogen 237 (1998) 245
Bacchus-Montabonel, M.C., see Talbi, D. 232 (1998) 267
Bacchus-Montabonel, M.C., see Honvault, P. 238 (1998) 401
Baddour-Hadjean, R., see Kagunya, W. 236 (1998) 225
Bagnich, S.A., Transport kinetics of triplet excitation in solid chrysene 237 (1998) 359
Baier, J., see Dahinten, T. 232 (1998) 239
Baltzer, P., L. Karlsson, B. Wannberg, D.M.P. Holland, M.A. MacDonald, M.A. Hayes and J.H.D. Eland, An experimental study of the valence shell photoelectron spectrum of the NO_2 molecule 237 (1998) 451
Baraldi, I., F. Momicchioli, G. Ponterini and D. Vanossi, Solvent effects within the CS INDO method. Geometrical distortion and solvatochromism of merocyanine dyes 238 (1998) 353
Barbier, C., see Lembarki, A. 232 (1998) 343
Barnes, I., see Klotz, B. 231 (1998) 289
Barroso, J., A. Costela, I. García-Moreno and R. Sastre, Wavelength dependence of the nonlinear absorption properties of laser dyes in solid and liquid solutions 238 (1998) 257
Barth, H.-D., K. Buchhold, S. Djafari, B. Reimann, U. Lommatzsch and B. Brutschy, Hydrogen bonding in (substituted benzene) \cdot (water) $_n$ clusters with $n \leq 4$ 239 (1998) 49
Bartussek, R., see Reimann, P. 235 (1998) 11
Barvík, I., C. Warns, T. Neidlinger and P. Reineker, Simulation of excitonic optical line shapes of cyclic molecular aggregates with 9 and 18 units: influence of quasi-static and dynamic disorder 240 (1999) 173
Basilevsky, M.V., I.V. Rostov and M.D. Newton, A frequency-resolved cavity model (FRCM) for treating equilibrium and non-equilibrium solvation energies 232 (1998) 189
Basilevsky, M.V., see Newton, M.D. 232 (1998) 201
Basilevsky, M.V., A.V. Soudackov and A.I. Voronin, Non-equilibrium interlevel transitions in condensed phase far away from the avoided crossing region 235 (1998) 281
Bässler, H., see Borsenberger, P.M. 234 (1998) 277
Bastida, A., J. Zuñiga, A. Requena, N. Halberstadt and J.A. Beswick, Competition between electronic and vibrational predissociation in $\text{Ar}-\text{I}_2(\text{B})$: a molecular dynamics with quantum transitions study 240 (1999) 229
Bauerle, S., see Gierczak, T. 231 (1998) 229
Baumfalk, R., see Menzel, C. 239 (1998) 287
Baumgärtel, H., see Locht, R. 233 (1998) 145

- Bauschlicher, Jr., C.W., Infrared spectra of polycyclic aromatic hydrocarbons: oxygen substitution 233 (1998) 29
- Bauschlicher, Jr., C.W. and S.R. Langhoff, Infrared spectra of polycyclic aromatic hydrocarbons: methyl substitution and loss of H 234 (1998) 79
- Bauschlicher, Jr., C.W., Infrared spectra of polycyclic aromatic hydrocarbons: nitrogen substitution 234 (1998) 87
- Becker, K.H., see Klotz, B. 231 (1998) 289
- Belić, D.S., see Poparić, G. 240 (1999) 283
- Belikov, A.E., M.M. Ahern and M.A. Smith, REMPI spectroscopy of internal state populations in HBr + Ar free jets: Rotational relaxation of HBr 234 (1998) 195
- Belikov, A.E., see Sharafutdinov, R.G. 233 (1998) 127
- Belinsky, M.I., High-order double exchange in mixed-valence [Fe(III)Fe(II)] cluster 240 (1999) 303
- Beltramo, G., C. Bilger, B. Pettinger and W. Schmickler, The second-harmonic response of single-crystal silver electrodes obtained with an interference method 238 (1998) 473
- Benderskii, V.A., E.V. Vetoshkin and H.P. Trommsdorff, Tunneling splittings in vibrational spectra of non-rigid molecules: III. Tunneling coordinate-dependent coupling between small amplitude motions 234 (1998) 153
- Benderskii, V.A. and E.V. Vetoshkin, Tunneling splittings in vibrational spectra of non-rigid molecules. IV. Kinematic couplings 234 (1998) 173
- Berezhkovskii, A.M., V.Yu. Zitserman, D.-Y. Yang and S.H. Lin, Reversible chemical reactions in slowly relaxing environments: Kramers' turnover of the rate constant 235 (1998) 201
- Berezhkovskii, A.M., see Talkner, P. 235 (1998) 131
- Berg, C., M. Beyer, U. Achatz, S. Joos, G. Niedner-Schatteburg and V.E. Bondybey, Stability and reactivity of hydrated magnesium cations 239 (1998) 379
- Berg, M.A. and H.W. Hubble, A viscoelastic continuum model of non-polar solvation. II. Vibrational dephasing in moderate to high-viscosity liquids and glasses 233 (1998) 257
- Berlin, Y.A., see Siebbeles, L.D.A. 238 (1998) 97
- Beržanskis, A., see Gaižauskas, E. 235 (1998) 123
- Beswick, J.A., see Bastida, A. 240 (1999) 229
- Beu, T.A., see Siebers, J.G. 239 (1998) 549
- Beust, R., N. Tyutyulkov, M. Rabinovitz and F. Dietz, Radical-substituted allenes as high-spin species and subunits of organic ferromagnets 240 (1999) 141
- Beyer, M., see Berg, C. 239 (1998) 379
- Bierbaum, V.M., see Frost, M.J. 231 (1998) 145
- Bieske, E.J., see Nizkorodov, S.A. 239 (1998) 369
- Bilger, C., see Beltramo, G. 238 (1998) 473
- Billard, I., see Bockstahl, F. 236 (1998) 393
- Billard, I., see Bouby, M. 240 (1999) 353
- Billing, G.D., see Adhikari, S. 238 (1998) 69
- Bini, R., J. Ebenhoch, M. Fanti, P.W. Fowler, S. Leach, G. Orlandi, Ch. Rüchardt, J.P.B. Sandall and F. Zerbetto, The vibrational spectroscopy of C₆₀H₃₆: An experimental and theoretical study 232 (1998) 75
- Blank, D.A., N. Hemmi, A.G. Suits and Y.T. Lee, A crossed molecular beam investigation of the reaction Cl + propane → HCl + C₃H₇ using VUV synchrotron radiation as a product probe 231 (1998) 261
- Blau, W.J., see Qureshi, F.M. 231 (1998) 87
- Blumen, A., see Sokolov, I.M. 235 (1998) 39

- Bockstahl, F., I. Billard, G. Duplâtre and A. Bonnenfant, Positronium formation and quenching in frozen and liquid solutions in octanol 236 (1998) 393
- Bodo, E., E. Buonomo, F.A. Gianturco, S. Kumar, A. Famulari, M. Raimondi and M. Sironi, Interaction anisotropy and quantum dynamics for vibrationally inelastic collisions of $\text{LiH}(^1\Sigma)$ with $\text{He}(^1S)$ 237 (1998) 315
- Bogár, F. and J. Ladik, Correlation corrected energy bands of nucleotide base stacks 237 (1998) 273
- Bol'shakov, B.V., see Grebenkin, S.Yu. 234 (1998) 239
- Bondybey, V.E., see Berg, C. 239 (1998) 379
- Bonnenfant, A., see Bockstahl, F. 236 (1998) 393
- Bonnenfant, A., see Bouby, M. 240 (1999) 353
- Bordes, B., F. Coletta, A. Ferrarini, F. Gottardi and P.L. Nordio, ^{13}C NMR relaxation in neutral and charged tetra-*n*-alkyl compounds 231 (1998) 51
- Börjesson, L.E.B., see Svedung, H. 236 (1998) 189
- Borrás-Almenar, J.J., E. Coronado, S.M. Ostrovsky, A.V. Palii and B.S. Tsukerblat, Localisation vs. delocalisation in the dimeric mixed-valence clusters in the generalised vibronic model. Magnetic manifestations 240 (1999) 149
- Borromeo, M., see Cattuto, C. 235 (1998) 51
- Borsenberger, P.M., W.T. Gruenbaum, U. Wolf and H. Bässler, Hole trapping in tri-*p*-tolylamine-doped poly(styrene) 234 (1998) 277
- Borsenberger, P.M., see Visser, S.A. 240 (1999) 197
- Bouby, M., I. Billard, A. Bonnenfant and G. Klein, Are the changes in the lifetime of the excited uranyl ion of chemical or physical nature? 240 (1999) 353
- Bougéard, D., see Ermoshin, V.A. 237 (1998) 333
- Boyd, I.D., see Longo, S. 238 (1998) 445
- Bradley, D.D.C., see Qureshi, F.M. 231 (1998) 87
- Bréchignac, P., see Parneix, P. 239 (1998) 121
- Brems, V., A simple analytical estimate of the bound-free Franck–Condon factors for a transition to a repulsive exponential potential in a diatomic molecule 238 (1998) 85
- Brenner, V., see Uridat, D. 239 (1998) 151
- Breton, J., see Iglesias-Groth, S. 237 (1998) 285
- Brey, J.J., see Drozdov, A.N. 235 (1998) 147
- Brickmann, J., see Gudowska-Nowak, E. 232 (1998) 247
- Brion, C.E., see Olney, T.N. 232 (1998) 211
- Brion, C.E., see Feng, R. 240 (1999) 371
- Broer, R., see de Graaf, C. 237 (1998) 59
- Brouwer, A.M., W.J. Buma, R. Caudano, M. Fanti, C.-A. Fustin, D.A. Leigh, A. Murphy, P. Rudolf, F. Zerbetto and J.M. Zwier, Experimental and theoretical studies of the low-lying electronic states of the simplest benzylic amide [2]catenane 238 (1998) 421
- Brutschy, B., see Lommatzsch, U. 234 (1998) 35
- Brutschy, B., see Barth, H.-D. 239 (1998) 49
- Buchhold, K., see Barth, H.-D. 239 (1998) 49
- Buck, U., see Kreil, J. 239 (1998) 459
- Buck, U., see Siebers, J.G. 239 (1998) 549
- Buma, W.J., see Brouwer, A.M. 238 (1998) 421
- Buntinx, G., see Didierjean, C. 237 (1998) 169
- Buonomo, E., see Clarke, N.J. 233 (1998) 9
- Buonomo, E., see Bodo, E. 237 (1998) 315
- Burkholder, J.B., see Gierczak, T. 231 (1998) 229

- Burshtein, A.I. and A.Yu. Sivachenko, Photochemical accumulation and recombination of ion pairs undergoing the singlet–triplet conversion 235 (1998) 257
- Burton, G.R., see Feng, R. 240 (1999) 371
- Burtsev, A.P., see Kolomiitsova, T.D. 238 (1998) 315
- Bylina, E.J., see Kummer, A.D. 237 (1998) 183
- Cabaleiro-Lago, E.M. and M.A. Ríos, An intermolecular potential function for Na^+ –acetonitrile obtained from ab initio calculations. Application to liquid simulations 236 (1998) 235
- Cai, Z.-L. and J.P. François, Ab initio study of the $X^2\Sigma^+$ and $A^2\Pi$ states of the SiO^+ cation including the effect of core correlation 234 (1998) 59
- Calhorda, M.J., see Lobo, R.F.M. 234 (1998) 265
- Caminati, W., P.G. Favero and B. Velino, Adducts of aromatic molecules with rare gases: rotational spectrum of pyrazole–argon 239 (1998) 223
- Caminati, W., see Melandri, S. 239 (1998) 229
- Cammi, R., see Champagne, B. 238 (1998) 153
- Campbell, E.E.B., R. Ehlich, G. Heusler, O. Knospe and H. Sprang, Capture dynamics in collisions between fullerene ions and rare gas atoms 239 (1998) 299
- Capobianco, J.A., see Misra, S.K. 240 (1999) 313
- Car, R., see Jimenez, S. 233 (1998) 343
- Caratti, G., R. Ferrando, R. Spadacini and G.E. Tommei, The Kramers problem in 2D-coupled periodic potentials 235 (1998) 157
- Cardin, F., see Moro, G.J. 235 (1998) 189
- Carles, S., see Desfrancois, C. 239 (1998) 475
- Carravetta, V., see Plashkevych, O. 232 (1998) 49
- Cascales, C., R. Sáez Puche and P. Porcher, Paramagnetic susceptibility simulations from crystal field effects on Nd^{3+} in magnesium borate $\text{MgNd}(\text{BO}_2)_5$ 240 (1999) 291
- Cassidei, L., see Petrella, G. 231 (1998) 31
- Castet, F., L. Ducasse and A. Fritsch, A Valence-Bond/Hartree–Fock method to determine the Hubbard transfer integrals in organic conductors 232 (1998) 37
- Castillejo, M., S. Couris, E. Lane, M. Martin and J. Ruiz, Laser photodissociation of ketene at 230 nm 232 (1998) 353
- Castleman Jr., A.W., see Poth, L. 239 (1998) 309
- Casu, M., see Marincola, F.C. 236 (1998) 301
- Cattuto, C., M. Borromeo and F. Marchesoni, Thermal decay of a metastable elastic string 235 (1998) 51
- Caudano, R., see Brouwer, A.M. 238 (1998) 421
- Cavalli, E., see Misra, S.K. 240 (1999) 313
- Cavell, R.G., see Neville, J.J. 238 (1998) 201
- Chakraborty, D., J. Park and M.C. Lin, Theoretical study of the $\text{OH} + \text{NO}_2$ reaction: formation of nitric acid and the hydroperoxyl radical 231 (1998) 39
- Chakraborty, D.K., see Polavarapu, P.L. 240 (1999) 1
- Chalaśiński, G., see Jakowski, J. 239 (1998) 573
- Champagne, B., B. Mennucci, M. Cossi, R. Cammi and J. Tomasi, An ab initio time-dependent Hartree–Fock study of solvent effects on the polarizability and second hyperpolarizability of polyacetylene chains within the polarizable continuum model 238 (1998) 153
- Chandra, A., Solvent effects on outersphere electron transfer reactions in mixed dipolar liquids 238 (1998) 285
- Chandra, A., see Senapati, S. 231 (1998) 65
- Chandra, A.K. and M.T. Nguyen, A density functional study of weakly bound hydrogen bonded complexes 232 (1998) 299

- Chang, Y. and C.A. Ordonez, Generalization of the Arrhenius relation and ionization reaction rates for carbon atoms and ions in plasmas 231 (1998) 27
- Chapman, D.M., F.J. Hompf, K. Müller-Dethlefs, E. Waterstradt, P. Hobza and V. Špirko, Structure and dynamics of the phenol-water-argon cation radical 239 (1998) 417
- Chaquin, P., see Hallou, A. 237 (1998) 251
- Chen, I.-C., see Jen, S.-H. 232 (1998) 131
- Chen, J.H., P.N. Wang, F.M. Li, Y.Q. Chen and Z.G. Wang, The first-order electric field-induced spectra: theory and experimental study of NO₂ 238 (1998) 165
- Chen, S.P., see Tsai, C.Y. 240 (1999) 191
- Chen, Y.Q., see Chen, J.H. 238 (1998) 165
- Cheng, P.-Y., see DeRose, P. 239 (1998) 235
- Chergui, M., see Jimenez, S. 233 (1998) 343
- Chesnut, D.B., Differential ring proton NMR shieldings and cyclic stabilization energies 231 (1998) 1
- Chesnut, D.B., see Dransfeld, A. 234 (1998) 69
- Chibisov, A.K. and H. Görner, Complexes of spiropyran-derived merocyanines with metal ions: relaxation kinetics, photochemistry and solvent effects 237 (1998) 425
- Cho, C.H., S. Singh and G.W. Robinson, Water anomalies and the double-well Takahashi model 232 (1998) 329
- Ciriaco, F., see Petrella, G. 231 (1998) 31
- Clarke, N.J., M. Sironi, M. Raimondi, S. Kumar, F.A. Gianturco, E. Buonomo and D.L. Cooper, Classical and quantum dynamics on the collinear potential energy surface for the reaction of Li with H₂ 233 (1998) 9
- Coleman, W.J., see Kummer, A.D. 237 (1998) 183
- Coletta, F., see Bordes, B. 231 (1998) 51
- Colominas, C., F.J. Luque, J. Teixidó and M. Orozco, Cavitation contribution to the free energy of solvation. Comparison of different formalisms in the context of MST calculations 240 (1999) 253
- Cong, S.-L., see Wang, M.-L. 238 (1998) 481
- Consalvo, D., see Storm, V. 237 (1998) 395
- Consalvo, D., see Storm, V. 239 (1998) 109
- Consalvo, D., see Spoerel, U. 239 (1998) 199
- Consolati, G., R. Rurali and M. Stefanetti, An experimental test on the distribution of positronium lifetimes in polymers 237 (1998) 493
- Continetti, R.E., see Hanold, K.A. 239 (1998) 493
- Cooper, D.L., see Clarke, N.J. 233 (1998) 9
- Cooper, G., see Olney, T.N. 232 (1998) 211
- Cooper, G., see Feng, R. 240 (1999) 371
- Cormack, A.J., see Yench, A.J. 238 (1998) 109
- Cormack, A.J., see Yench, A.J. 238 (1998) 133
- Coronado, E., see Borrás-Almenar, J.J. 240 (1999) 149
- Cossi, M., see Champagne, B. 238 (1998) 153
- Costela, A., see López Arbeloa, F. 236 (1998) 331
- Costela, A., see Barroso, J. 238 (1998) 257
- Couris, S., see Castillejo, M. 232 (1998) 353
- Cundari, T.R., H.A. Kurtz and T. Zhou, Modeling nonlinear optical properties of inorganic complexes. Counterion effects 240 (1999) 205
- Cybulski, S.M., see Jakowski, J. 239 (1998) 573

- Dagdigian, P.J., see Yang, X. 239 (1998) 207
- Dahinten, T., J. Baier and A. Seilmeier, Vibrational energy transfer processes in dye molecules after ultrafast excitation of skeletal modes 232 (1998) 239
- Dai, H.-L., see DeRose, P. 239 (1998) 235
- De Almeida, W.B., see Resende, S.M. 238 (1998) 11
- De Alti, G., see Fronzoni, G. 232 (1998) 9
- De Boeij, W.P., M.S. Pshenichnikov and D.A. Wiersma, Heterodyne-detected stimulated photon echo: applications to optical dynamics in solution 233 (1998) 287
- Decleva, P., see Fronzoni, G. 232 (1998) 9
- Decleva, P., see Venuti, M. 234 (1998) 95
- Decleva, P., see Fronzoni, G. 237 (1998) 21
- Dedonder-Lardeux, C., see Martrenchard, S. 239 (1998) 331
- De Graaf, C., W.A. de Jong, R. Broer and W.C. Nieuwpoort, Theoretical study of the crystal field excitations in CoO 237 (1998) 59
- De Groot, F.M.F., see Hu, Z. 232 (1998) 63
- De Jong, W.A., see de Graaf, C. 237 (1998) 59
- Delaney, N., see Faeder, J. 239 (1998) 525
- Delon, A., S. Heilliette and R. Jost, 'Anomalous' density of states and rotational selection rules of loosely bound states of NO₂ 238 (1998) 465
- Deng, H., Z. Lu, Y. Shen, H. Mao and H. Xu, Improvement in photoelectric conversion of a phthalocyanine-sensitized TiO₂ electrode by doping with porphyrin 231 (1998) 95
- Denifl, G., see Muigg, D. 239 (1998) 409
- Denzer, W., G. Hancock, J.C. Pinot de Moira and P.L. Tyley, Spin-forbidden dissociation of ozone in the Huggins bands 231 (1998) 109
- DeRose, P., P.-Y. Cheng, B. Xue, S.-S. Ju and H.-L. Dai, Isomeric structures, large amplitude intermolecular motions and electronic relaxation of the propynal–Ar complex 239 (1998) 235
- Desfrancois, C., V. Périquet, S. Carles, J.P. Schermann and L. Adamowicz, Neutral and negatively-charged formamide, N-methylformamide and dimethylformamide clusters 239 (1998) 475
- Detken, A., P. Schiebel, M.R. Johnson, H. Zimmermann and U. Haeberlen, Rotational tunneling of methyl groups in the hydroquinone/acetonitrile clathrate: A combined deuteron NMR, INS, and computational study 238 (1998) 301
- Devoret, M.H., see Turlot, E. 235 (1998) 47
- De Waele, V., see Didierjean, C. 237 (1998) 169
- Dickebohmer, M.S., see Gutmann, M. 239 (1998) 317
- Didierjean, C., V. De Waele, G. Buntinx and O. Poizat, The structure of the lowest excited singlet (S₁) state of 4,4'-bipyridine: a picosecond time-resolved Raman analysis 237 (1998) 169
- Dietz, F., see Beust, R. 240 (1999) 141
- Di Marco, P., see Kalinowski, J. 237 (1998) 233
- Dimicoli, I., see Uridat, D. 239 (1998) 151
- Dimicoli, I., see Martrenchard, S. 239 (1998) 331
- Ding, S., see Guan, D. 233 (1998) 35
- Djafari, S., see Barth, H.-D. 239 (1998) 49
- Djahandideh, D., see Janda, K.C. 239 (1998) 177
- Doktorov, A.B., see Jenkins, O.B. 234 (1998) 121
- Domcke, W., see Sobolewski, A.L. 232 (1998) 257
- Domcke, W., see Wolfseder, B. 233 (1998) 323
- Domcke, W., see Sudholt, W. 240 (1999) 9
- Donovan, R.J., see Yench, A.J. 238 (1998) 109

- Donovan, R.J., see Yench, A.J. 238 (1998) 133
Dopfer, O., see Olkhov, R.V. 239 (1998) 393
Dötz, K.H., see Engemann, C. 237 (1998) 471
Dransfeld, A. and D.B. Chesnut, An ab initio study of NMR isotropic shielding bond length derivatives in phosphorus compounds 234 (1998) 69
Dreizler, H., see Storm, V. 237 (1998) 395
Dreizler, H., see Storm, V. 239 (1998) 109
Drozov, A.N. and J.J. Brey, On the role of the energy loss in turnover theories of activated rate processes 235 (1998) 147
Duan, Y., Chemical bonding and magnetic properties of the high-spin molecule $[\text{Mn}_{12}\text{O}_{12}(\text{HCOO})_{16}(\text{H}_2\text{O})_4]$ 238 (1998) 407
Ducasse, L., see Castet, F. 232 (1998) 37
Duhoo, T., see Lemoine, D. 238 (1998) 59
Duncan, M.A., see France, M.R. 239 (1998) 447
Duplâtre, G., see Bockstahl, F. 236 (1998) 393
Duppen, K., see Steffen, T. 233 (1998) 267
Duran, M., see Forés, M. 234 (1998) 1

Ebata, T., K. Nagao and N. Mikami, Mode-dependent anharmonic coupling between OH stretching and intermolecular vibrations of the hydrogen-bonded clusters of phenol 231 (1998) 199
Ebenhoch, J., see Bini, R. 232 (1998) 75
Echt, O., see Muigg, D. 239 (1998) 409
Edwards, M.A. and J.F. Hershberger, Kinetics of the $\text{CN} + \text{CH}_2\text{CO}$ and $\text{NCO} + \text{CH}_2\text{CO}$ reactions 234 (1998) 231
Egorov, S.A., see Everitt, K.F. 235 (1998) 115
Ehlich, R., see Campbell, E.E.B. 239 (1998) 299
Eilmes, A. and P. Petelenz, Model calculations of local exciton levels in the C_{60} fullerene crystals doped with endohedral fullerenes $\text{M}@\text{C}_{60}$ 237 (1998) 67
Eland, J.H.D., see Hochlaf, M. 234 (1998) 249
Eland, J.H.D. and L. Karlsson, Dissociative photoionisation of NO_2 up to 26 eV 237 (1998) 139
Eland, J.H.D., see Baltzer, P. 237 (1998) 451
Endo, N., see Shirota, H. 238 (1998) 487
Engels, B., see Perić, M. 231 (1998) 105
Engels, B., see Salhi-Benachenhou, N. 236 (1998) 53
Engels, B., see Perić, M. 238 (1998) 33
Engels, B., see Perić, M. 238 (1998) 47
Engemann, C., J. Hormes, A. Longen and K.H. Dötz, An X-ray absorption near edge spectroscopy (XANES) study on organochromium complexes at the Cr K-edge 237 (1998) 471
Engleitner, S., see Wolfseder, B. 233 (1998) 323
Engström, M., B. Minaev, O. Vahtras and H. Ågren, Linear response calculations of electronic g -factors and spin-rotational coupling constants for diatomic molecules with a triplet ground state 237 (1998) 149
Ermisch, K., see Lindner, J. 238 (1998) 329
Ermoshin, V.A., A.K. Kazansky, K.S. Smirnov and D. Bougeard, The energy relaxation of Si-H vibration in the H/Si(111) system. Relaxation rate and potential energy surface anharmonicity 237 (1998) 333
Esteve, D., see Turlot, E. 235 (1998) 47
Ettischer, I., see Kreil, J. 239 (1998) 459

- Evans, M., see Hsu, C.-W. 231 (1998) 121
- Everitt, K.F., S.A. Egorov and J.L. Skinner, Vibrational energy relaxation in liquid oxygen 235 (1998) 115
- Faeder, J., N. Delaney, P.E. Maslen and R. Parson, Modeling structure and dynamics of solvated molecular ions: Photodissociation and recombination in $I_2^-(CO_2)_n$ 239 (1998) 525
- Fahr, A., P. Hassanzadeh and D.B. Atkinson, Ultraviolet absorption spectrum and cross-sections of vinyl (C_2H_3) radical in the 225–238 nm region 236 (1998) 43
- Famulari, A., M. Raimondi, M. Sironi and E. Gianinetti, Hartree–Fock limit properties of the water dimer in absence of BSSE 232 (1998) 275
- Famulari, A., M. Raimondi, M. Sironi and E. Gianinetti, Ab initio MO–VB study of water dimer 232 (1998) 289
- Famulari, A., see Bodo, E. 237 (1998) 315
- Fanti, M., see Bini, R. 232 (1998) 75
- Fanti, M., see Brouwer, A.M. 238 (1998) 421
- Favaro, G., see Romani, A. 237 (1998) 413
- Favero, P.G., see Caminati, W. 239 (1998) 223
- Favero, P.G., see Melandri, S. 239 (1998) 229
- Fedoseev, V.G., see Kolomiitsova, T.D. 238 (1998) 315
- Feigel'man, M.V. and A.I. Larkin, Quantum superconductor–metal transition in a 2D proximity-coupled array 235 (1998) 107
- Feller, K.-H., see Gaižauskas, E. 235 (1998) 123
- Feng, K., see Xiao, C. 237 (1998) 73
- Feng, R., G. Cooper, G.R. Burton, C.E. Brion and L. Avaldi, Absolute photoabsorption oscillator strengths by electron energy loss methods: the valence and S 2p and 2s inner shells of sulphur dioxide in the discrete and continuum regions (3.5–260 eV) 240 (1999) 371
- Ferguson, D.M., see Paterlini, M.G. 236 (1998) 243
- Ferrando, R., see Caratti, G. 235 (1998) 157
- Ferrarini, A., see Bordes, B. 231 (1998) 51
- Fidder, H., G.J.S. Fowler, C.N. Hunter and V. Sundström, Optical dephasing in photosynthetic pigment–protein complexes 233 (1998) 311
- Fiss, J.A., L. Zhu, K. Suto, G. He and R.J. Gordon, Mechanism of the coherent control of the photoionization and photodissociation of HI and DI 233 (1998) 335
- Flament, J.P., see Tadjeddine, M. 240 (1999) 39
- Fleming, G.R., see Tokmakoff, A. 233 (1998) 231
- Ford, J.V., see Poth, L. 239 (1998) 309
- Forés, M., M. Duran and M. Solà, Intramolecular proton transfer in the ground and the two lowest-lying singlet excited states of 1-amino-3-propenal and related species 234 (1998) 1
- Forrest, S.R., see Kiselev, S.A. 238 (1998) 365
- Fowler, G.J.S., see Fidder, H. 233 (1998) 311
- Fowler, P.W., see Bini, R. 232 (1998) 75
- Fox, R.F., see Thorwart, M. 235 (1998) 61
- France, M.R., S.H. Pullins and M.A. Duncan, Photodissociation of $Mg^+-(CH_3OH)_N$ complexes: evidence for the onset of solvation 239 (1998) 447
- Francisco, J.S., The mechanism of the $CH_3O + CO$ reaction and the stability of the CH_3OCO radical 237 (1998) 1
- François, J.P., see Cai, Z.-L. 234 (1998) 59
- Freund, H.-J., see Thiel, S. 236 (1998) 263

- Fritsch, A., Non-orthogonal orbitals for localized electrons. I. The Spin-Coupled wavefunction 238 (1998) 373
Fritsch, A., see Castet, F. 232 (1998) 37
Fronzoni, G., M. Stener, P. Decleva and G. De Alti, Theoretical study of the Cl 1s and 2p near edge photoabsorption spectra of HCl by accurate ab-initio configuration interaction and density functional approaches 232 (1998) 9
Fronzoni, G. and P. Decleva, Ab-initio CI calculations of the Cl 1s and Cl 1s and 2p core excitation spectra of the freon molecules: CCl₄, CFCI₃, CF₂Cl₂ and CF₃Cl 237 (1998) 21
Frost, M.J., S. Kato, V.M. Bierbaum and S.R. Leone, Reactions of N₂⁺(*v*) with CO and NO at thermal energy 231 (1998) 145
Fuß, W., S. Lochbrunner, A.M. Müller, T. Schikarski, W.E. Schmid and S.A. Trushin, Pathway approach to ultrafast photochemistry: potential surfaces, conical intersections and isomerizations of small polyenes 232 (1998) 161
Fustin, C.-A., see Brouwer, A.M. 238 (1998) 421

Gaižauskas, E., A. Beržanskis and K.-H. Feller, Effects of non-Markovian relaxation in the femtosecond differential absorption spectra 235 (1998) 123
Galembeck, S.E., see Alemán, C. 232 (1998) 151
Galembeck, S.E., see Alemán, C. 233 (1998) 85
Gang, J., M.J. Pilling and S.H. Robertson, Monte Carlo calculation of partition functions for straight chain alkanes 231 (1998) 183
Garay, M., C.A. Rinaldi, J.M. Orea and A. González Ureña, On the electronic energy disposal of calcium excited atom reactions with halogen-containing compounds: Electronic branching ratio and spin-orbit state populations 236 (1998) 343
García, J.I., see Alvira, E. 240 (1999) 101
García-Moreno, I., see López Arbeloa, F. 236 (1998) 331
García-Moreno, I., see Barroso, J. 238 (1998) 257
Gargaud, M., see Honvault, P. 238 (1998) 401
Garnier, F., see Kalinowski, J. 237 (1998) 233
Gelin, M.F., A Keilson-Storer type collision kernel for rotation-translation coupling 240 (1999) 265
Gerasimov, I., see Yang, X. 239 (1998) 207
Gianinetti, E., see Famulari, A. 232 (1998) 275
Gianinetti, E., see Famulari, A. 232 (1998) 289
Gianturco, F.A., see Clarke, N.J. 233 (1998) 9
Gianturco, F.A., see Bodo, E. 237 (1998) 315
Gierczak, T., J.B. Burkholder, S. Bauerle and A.R. Ravishankara, Photochemistry of acetone under tropospheric conditions 231 (1998) 229
Gilliams, B., D. Vandenbroucke and C. Görrler-Walrand, Modelling the substitution effects of several rhodium(III) transition metal complexes using the angular overlap model 237 (1998) 91
Gingell, J.M., G. Marston, N.J. Mason, H. Zhao and M.R.F. Siggel, On the electronic spectroscopy of benzyl alcohol 237 (1998) 443
Girardet, C., see Iglesias-Groth, S. 237 (1998) 285
Gislason, E.A., see Song, J.-B. 237 (1998) 159
Gole, J.L., see McQuaid, M.J. 234 (1998) 297
González Ureña, A., see Garay, M. 236 (1998) 343
Gordon, R.J., see Alexander, M.H. 231 (1998) 331
Gordon, R.J., see Fiss, J.A. 233 (1998) 335
Gorecka, J.N., see Gorecki, J. 240 (1999) 215

- Gorecki, J. and J.N. Gorecka, On the nonequilibrium effects in thermally activated reactions $A + A \rightleftharpoons B + B \rightleftharpoons C + C$ 240 (1999) 215
- Görller-Walrand, C., see Gilliams, B. 237 (1998) 91
- Görner, H., see Chibisov, A.K. 237 (1998) 425
- Gottardi, F., see Bordes, B. 231 (1998) 51
- Gould, I.R., see Scholes, G.D. 234 (1998) 21
- Grabert, H., see Turlot, E. 235 (1998) 47
- Graf, P. and A. Nitzan, Numerical simulations of solvation in simple polar fluids: dependence on the thermodynamic state below and above the critical point 235 (1998) 297
- Grebenkin, S.Yu. and B.V. Bol'shakov, Light induced *cis-trans* isomerization of azo compounds in polymethyl methacrylate 234 (1998) 239
- Grégoire, G., see Martrenchard, S. 239 (1998) 331
- Griffiths, I.W., D.E. Parry and F.M. Harris, Vertical double ionization of the sulphur dioxide molecule 238 (1998) 21
- Grifoni, M., L. Hartmann and P. Hänggi, Erratum to "Dissipative tunneling with periodic polychromatic driving: Exact results and tractable approximations" [Chem. Phys. 217 (1997) 167] 232 (1998) 371
- Grigorenko, B.L., A.V. Nemukhin and V.A. Apkarian, Towards quantitative diatomics-in-molecules model for the water molecule 232 (1998) 321
- Gruenbaum, W.T., see Borsenberger, P.M. 234 (1998) 277
- Gruenbaum, W.T., see Visser, S.A. 240 (1999) 197
- Gruenloh, C.J., see Hagemeister, F.C. 239 (1998) 83
- Gu, L., see Guan, D. 233 (1998) 35
- Guan, D., X. Yi, S. Ding, L. Gu and J.A. Olson, Charge transfer in gas-surface scattering: the three electronic state system 233 (1998) 35
- Gudowska-Nowak, E., G. Papp and J. Brickmann, Bridged-assisted electron transfer. Random matrix theory approach 232 (1998) 247
- Guest, M.F., see Palmer, M.H. 238 (1998) 179
- Guo, J.-H., see Magnuson, M. 237 (1998) 295
- Gutmann, M., J.M. Janello and M.S. Dickebohm, Ultrafast dynamics of transition metal carbonyls. II. Picosecond evaporation after photodissociation of $\text{Cr}(\text{CO})_6 \cdot (\text{CH}_3\text{OH})_n$ heteroclusters at 280 nm 239 (1998) 317
- Haarer, D., see Müller, J. 237 (1998) 483
- Haeblerlen, U., see Detken, A. 238 (1998) 301
- Hagemeister, F.C., C.J. Gruenloh and T.S. Zwier, Resonant ion-dip infrared spectroscopy of benzene-(water)_n-(methanol)_m clusters with $n + m = 4, 5$ 239 (1998) 83
- Halberstadt, N., see Janda, K.C. 239 (1998) 177
- Halberstadt, N., see Bastida, A. 240 (1999) 229
- Hall, R.I., see Hochlaf, M. 234 (1998) 249
- Hallou, A., L. Schriver-Mazzuoli, A. Schriver and P. Chaquin, Matrix photochemistry of nitrosyl chloride. Interconversion of ClNO and ClON species by irradiation and tunneling effect 237 (1998) 251
- Han, K.-L., see Wang, M.-L. 236 (1998) 387
- Han, K.-L., see Wang, M.-L. 238 (1998) 481
- Hancock, G., see Denzer, W. 231 (1998) 109
- Hänggi, P., see Grifoni, M. 232 (1998) 371
- Hänggi, P., see Reimann, P. 235 (1998) 11

- Hänggi, P., see Shao, J. 235 (1998) 81
- Hanold, K.A. and R.E. Continetti, Photoelectron–photofragment coincidence studies of the dissociative photodetachment of O_4^- 239 (1998) 493
- Hanrath, M., see Perić, M. 238 (1998) 33
- Hansen, K., see Weber, J.M. 239 (1998) 271
- Harris, F.M., see Griffiths, I.W. 238 (1998) 21
- Hartke, B., M. Schütz and H.-J. Werner, Improved intermolecular water potential from global geometry optimization of small water clusters using local MP2 239 (1998) 561
- Hartmann, L., see Grifoni, M. 232 (1998) 371
- Hartmann, M., A. Lindinger, J.P. Toennies and A.F. Vilesov, Laser-induced fluorescence spectroscopy of van der Waals complexes of tetracene– Ar_N ($N \leq 5$) and pentacene–Ar within ultracold liquid He droplets 239 (1998) 139
- Hartung, E., see Kiselev, S.A. 238 (1998) 365
- Hartung, S., see Kück, S. 240 (1999) 387
- Hassanzadeh, P., see Fahr, A. 236 (1998) 43
- Hawlicka, E. and D. Swiatla-Wojcik, Molecular dynamics studies of NaCl solutions in methanol–water mixtures. An effect of NaCl on hydrogen bonded network 232 (1998) 361
- Hayes, M.A., see Rennie, E.E. 236 (1998) 365
- Hayes, M.A., see Baltzer, P. 237 (1998) 451
- Hayes, S.C., see Philpott, M.J. 236 (1998) 207
- He, G., see Fiss, J.A. 233 (1998) 335
- He, G.-Z., see Wang, M.-L. 236 (1998) 387
- He, G.-Z., see Wang, M.-L. 238 (1998) 481
- Hedstrom, J.F., see Pauls, S.W. 237 (1998) 205
- Heilliette, S., see Delon, A. 238 (1998) 465
- Heilweil, E.J., see Kleiman, V.D. 233 (1998) 207
- Heimann, P., see Hsu, C.-W. 231 (1998) 121
- Helm, R.M. and H.J. Neusser, Highly resolved UV spectroscopy of clusters: isotope substitution studies of hydrogen-bonded phenol · water 239 (1998) 33
- Hemmerling, B., see Kouzov, A.P. 236 (1998) 15
- Hemmi, N., see Blank, D.A. 231 (1998) 261
- Henari, F.Z., see Qureshi, F.M. 231 (1998) 87
- Hering, P., see Jacoby, C. 239 (1998) 23
- Herman, M.F., see Velev, P. 240 (1999) 241
- Hernandez, R. and G.A. Voth, Quantum time correlation functions and classical coherence 233 (1998) 243
- Hershberger, J.F., see Edwards, M.A. 234 (1998) 231
- Heryadi, D., see McKellar, A.J. 238 (1998) 1
- Heusler, G., see Campbell, E.E.B. 239 (1998) 299
- Hirota, E., see Kawaguchi, K. 231 (1998) 193
- Hishikawa, A., A. Iwamae, K. Hoshina, M. Kono and K. Yamanouchi, Coulomb explosion dynamics of N_2 in intense laser field by mass-resolved momentum imaging 231 (1998) 315
- Hitchcock, A.P., see Neville, J.J. 238 (1998) 201
- Hobza, P., see Chapman, D.M. 239 (1998) 417
- Hochlaf, M., R.I. Hall, F. Penent, J.H.D. Eland and P. Lablanquie, Investigation of the CS_2^{2+} dication using threshold photoelectrons coincidence spectroscopy 234 (1998) 249
- Holland, D.M.P., see Rennie, E.E. 236 (1998) 365
- Holland, D.M.P., see Baltzer, P. 237 (1998) 451

- Holmlid, L., Classical energy calculations with electron correlation of condensed excited states — Rydberg Matter 237 (1998) 11
- Hompf, F.J., see Chapman, D.M. 239 (1998) 417
- Honvault, P., M.C. Bacchus-Montabonel, M. Gargaud and R. McCarroll, Charge transfer between Si^{3+} and helium at thermal and low energies 238 (1998) 401
- Hopkirk, A., see Yench, A.J. 238 (1998) 109
- Hopkirk, A., see Yench, A.J. 238 (1998) 133
- Horie, K., see Shirota, H. 238 (1998) 487
- Hormes, J., see Engemann, C. 237 (1998) 471
- Horsburgh, L.E., see Magnuson, M. 237 (1998) 295
- Hoshina, K., see Hishikawa, A. 231 (1998) 315
- Hotop, H., see Weber, J.M. 239 (1998) 271
- Hotop, H., see Kreil, J. 239 (1998) 459
- Hottmann, K., see Locht, R. 233 (1998) 145
- Hsu, C.-W., M. Evans, S. Stimson, C.Y. Ng and P. Heimann, High-resolution photoelectron spectroscopy using multibunch synchrotron radiation: rotational-resolved photoelectron bands of $\text{O}_2^+(\text{b}^4\Sigma_g^-, \nu^+)$ 231 (1998) 121
- Hsu, J.-P. and B.-T. Liu, Electrical interaction between two spherical particles covered by an ion-penetrable charged membrane 236 (1998) 63
- Hsu, J.-P., see Kuo, Y.-C. 236 (1998) 1
- Hsu, T.-J., see Jen, S.-H. 232 (1998) 131
- Hu, Z., G. Kaundl, S.A. Warda, D. Reinen, F.M.F. de Groot and B.G. Müller, On the electronic structure of Cu(III) and Ni(III) in $\text{La}_2\text{Li}_{1/2}\text{Cu}_{1/2}\text{O}_4$, $\text{Nd}_2\text{Li}_{1/2}\text{Ni}_{1/2}\text{O}_4$, and Cs_2KCuF_6 232 (1998) 63
- Huang, J.-H., see Wang, M.-L. 236 (1998) 387
- Huang, M.-B., see Salhi-Benachenh, N. 236 (1998) 53
- Huang, W., Z. Yu and Y. Zhang, Reactions of solid glycine induced by keV ion irradiation 237 (1998) 223
- Hubble, H.W., see Berg, M.A. 233 (1998) 257
- Huisken, F., S. Mohammad-Pooran and O. Werhahn, Vibrational spectroscopy of single methanol molecules attached to liquid water clusters 239 (1998) 11
- Hunter, C.N., see Fidler, H. 233 (1998) 311
- Hurley, S.M., see Poth, L. 239 (1998) 309
- Iglesias-Groth, S., J. Breton and C. Girardet, Structure of the Van der Waals rare gas- C_{60} exohedral complexes $[(\text{C}_{60})(\text{RG})_n; n = 1, 2]$ 237 (1998) 285
- Ikawa, S.-i., see Yasuda, T. 238 (1998) 173
- Ikushima, Y. and M. Arai, Raman spectroscopy study on the dynamic behavior of nitrate anion in zinc nitrate solution at high temperatures and pressure 238 (1998) 455
- Ilyukhin, A.A., see Sharafutdinov, R.G. 233 (1998) 127
- Inokuchi, Y., see Ohashi, K. 239 (1998) 429
- Inomata, S., see Zils, R. 231 (1998) 303
- Isber, S., see Misra, S.K. 240 (1999) 313
- Ishida, N., see Sato, K. 237 (1998) 195
- Ishiki, H.M., see Alemán, C. 233 (1998) 85
- Ishimi, H., see Tsuji, M. 236 (1998) 319
- Ishiwata, T., see Kawaguchi, K. 231 (1998) 193
- Itkin, A.L., On the dependence of a critical supersaturation on pressure of a two-component background gas in a diffusion cloud chamber 238 (1998) 273

- Iwamae, A., see Hishikawa, A. 231 (1998) 315
 Iwasaki, A., see Sato, K. 237 (1998) 195
 Iwata, S., see Ornellas, F.R. 232 (1998) 95
 Izvekov, V., see Kovács, A. 238 (1998) 231
- Jackson, N.A., C.J. Randall and K.G. McKendrick, Polarisation effects in electronically inelastic collisions: $\text{SiFC}^2\Delta + \text{H}_2 \rightarrow \text{SiFB}^2\Sigma^+ + \text{H}_2$ 233 (1998) 45
 Jacoby, C., P. Hering, M. Schmitt, W. Roth and K. Kleinermanns, Investigations of OH-N- and NH-O-type hydrogen-bonded clusters by UV laser spectroscopy 239 (1998) 23
 Jacoby, Ch., see Roth, W. 239 (1998) 1
 Jakowski, J., G. Chałasiński, M.M. Szczeniński and S.M. Cybulski, Many-body exchange effects in clusters of rare gases with a chromophore: He_2CO_2 239 (1998) 573
 Jalkanen, K.J., see Knapp-Mohammady, M. 240 (1999) 63
 Janda, K.C., D. Djahandideh, O. Roncero and N. Halberstadt, The $\text{B} \leftarrow \text{X}$ spectrum of ArCl_2 : linear and perpendicular isomers 239 (1998) 177
 Janello, J.M., see Gutmann, M. 239 (1998) 317
 Janzen, Ch., see Roth, W. 239 (1998) 1
 Jelezko, F., see Walla, P.J. 233 (1998) 117
 Jen, S.-H., T.-J. Hsu and I.-C. Chen, Fluorescence lifetime of rovibrational states of h_4 -acetaldehyde and spectra of d_4 -acetaldehyde 232 (1998) 131
 Jenkins, O.B. and A.B. Doktorov, The steady-state Green's function theory in monomolecular reactions. II. Effects of solvent dynamics and non-equilibrium initial distributions in reactions on position-dependent transition regions 234 (1998) 121
 Jimenez, S., A. Pasquarello, R. Car and M. Chergui, Dynamics of structural relaxation upon Rydberg excitation of an impurity in an Ar crystal 233 (1998) 343
 Johansson, N., see Magnuson, M. 237 (1998) 295
 Johari, G.P., see Wasylyshyn, D.A. 237 (1998) 345
 Johnson, C.A.F., see Rennie, E.E. 236 (1998) 365
 Johnson, C.K., see Pauls, S.W. 237 (1998) 205
 Johnson, M.A., see Ayotte, P. 239 (1998) 485
 Johnson, M.R., see Detken, A. 238 (1998) 301
 Johnston, R.L., see Lloyd, L.D. 236 (1998) 107
 Jones, M.R., see Vos, M.H. 233 (1998) 179
 Jones, W., see Kagunya, W. 236 (1998) 225
 Joos, S., see Berg, C. 239 (1998) 379
 Jordan, K.D., see Pedulla, J.M. 239 (1998) 593
 Jordanides, X.J., see Tokmakoff, A. 233 (1998) 231
 Jorge, F.E. and R.F. Martins, Accurate universal basis set for H through Xe for Hartree-Fock calculations 233 (1998) 1
 Jost, R., see Delon, A. 238 (1998) 465
 Jouvét, C., see Martrenchard, S. 239 (1998) 331
 Ju, S.-S., see DeRose, P. 239 (1998) 235
 Jug, K., see Wichmann, D. 236 (1998) 87
 Jung, P., see Thorwart, M. 235 (1998) 61
 Jürgensen, A., see Neville, J.J. 238 (1998) 201
 Jursic, B.S., Complete basis set ab initio study of monocomplexation of aluminum with H_2O , NH_3 , and HF 237 (1998) 51

- Kadashchuk, A., N. Ostapenko, V. Zaika and S. Nešpùrek, Low-temperature thermoluminescence in poly(methyl-phenylsilylene) 234 (1998) 285
- Kagunya, W., R. Baddour-Hadjean, F. Kooli and W. Jones, Vibrational modes in layered double hydroxides and their calcined derivatives 236 (1998) 225
- Kaindl, G., see Hu, Z. 232 (1998) 63
- Kalinowski, J., W. Stampor, P. Di Marco and F. Garnier, Photogeneration of charge in solid films of α -sexithiophene 237 (1998) 233
- Kapala, J., S. Roszak, I. Lisek and M. Miller, Mass spectrometric and theoretical study of the mixed complex $\text{NaCeCl}_4(\text{g})$ 238 (1998) 221
- Kar, A.K., see Qureshi, F.M. 231 (1998) 87
- Karlsson, L., see Eland, J.H.D. 237 (1998) 139
- Karlsson, L., see Baltzer, P. 237 (1998) 451
- Katayanagi, H., N. Yonekura and T. Suzuki, C–Br bond rupture in 193 nm photodissociation of vinyl bromide 231 (1998) 345
- Kato, S., see Frost, M.J. 231 (1998) 145
- Kato, S., see Takami, A. 231 (1998) 215
- Kawaguchi, K., T. Ishiwata, E. Hirota and I. Tanaka, Infrared spectroscopy of the NO_3 radical 231 (1998) 193
- Kawakami, Y., see Moriyama, M. 231 (1998) 205
- Kawasaki, M., see Takahashi, K. 231 (1998) 171
- Kazansky, A.K., see Ermoshin, V.A. 237 (1998) 333
- Kearley, G.J., see Line, C.M.B. 234 (1998) 207
- Keresztury, G., see Kovács, A. 238 (1998) 231
- Kharlamov, B.M., see Müller, J. 237 (1998) 483
- Khodykin, O.V., see Müller, J. 237 (1998) 483
- Kikuchi, O., see Yagi, T. 232 (1998) 1
- Kim, J., see Ayotte, P. 239 (1998) 485
- Kimura, K., see Tanaka, D. 239 (1998) 437
- King, G.C., see Yench, A.J. 238 (1998) 109
- King, G.C., see Yench, A.J. 238 (1998) 133
- Kirkwood, J.C., see Ulness, D.J. 240 (1999) 109
- Kiselev, S.A., E. Hartung, Z.G. Soos, S.R. Forrest and V.M. Agranovich, Cold photoconductivity in a system of interacting charge-transfer excitons at a donor–acceptor interface 238 (1998) 365
- Kitahama, Y. and H. Murai, The study on the magnetic field effect and the microwave effect on the photoconductivity observed in the photolysis of N,N,N',N' -tetramethyl-*p*-phenylenediamine: theoretical calculation trial by the stochastic Liouville equation 238 (1998) 429
- Kleiman, V.D., S.M. Arrivo, J.S. Melinger and E.J. Heilweil, Controlling condensed-phase vibrational excitation with tailored infrared pulses 233 (1998) 207
- Klein, G., see Bouby, M. 240 (1999) 353
- Kleinerhanns, K., see Roth, W. 239 (1998) 1
- Kleinerhanns, K., see Jacoby, C. 239 (1998) 23
- Klochikhin, V.L., see Trakhtenberg, L.I. 232 (1998) 175
- Klotz, B., I. Barnes and K.H. Becker, New results on the atmospheric photooxidation of simple alkylbenzenes 231 (1998) 289
- Klüner, T., see Thiel, S. 236 (1998) 263
- Knapp-Mohammady, M., K.J. Jalkanen, F. Nardi, R.C. Wade and S. Suhai, L-Alanyl-L-alanine in the zwitterionic state: structures determined in the presence of explicit water molecules and with continuum models using density functional theory 240 (1999) 63

- Knospe, O., see Campbell, E.E.B. 239 (1998) 299
- Koch, H., see Sauer, S.P.A. 238 (1998) 385
- Koda, S., see Takami, A. 231 (1998) 215
- Kolomiitsova, T.D., A.P. Burtsev, V.G. Fedoseev and D.N. Shchepkin, Manifestation of interaction of the transition dipole moments in IR spectra of low-temperature liquids and solutions in liquefied noble gases 238 (1998) 315
- Kompa, C., see Kummer, A.D. 237 (1998) 183
- Kono, M., see Hishikawa, A. 231 (1998) 315
- Kooli, F., see Kagunya, W. 236 (1998) 225
- Korolkov, M.V. and B. Schmidt, Vibrationally state-selective laser pulse control of electronic branching in OH ($X^2\Pi/A^2\Sigma^+$) photoassociation 237 (1998) 123
- Kostur, M., see Kula, J. 235 (1998) 27
- Kosugi, N., see Neville, J.J. 238 (1998) 201
- Kouzov, A.P., D.N. Kozlov and B. Hemmerling, CARS studies of bending states of CO₂: evidence of collisional rotational transitions with odd ΔJ 236 (1998) 15
- Kovács, A., V. Izvekov, G. Keresztury and G. Pongor, Vibrational analysis of 2-nitrophenol. A joint FT-IR, FT-Raman and scaled quantum mechanical study 238 (1998) 231
- Kozlov, D.N., see Kouzov, A.P. 236 (1998) 15
- Krause, J.L., see Skodje, R.T. 240 (1999) 129
- Kreil, J., M.-W. Ruf, H. Hotop, I. Ettischer and U. Buck, Threshold electron attachment and electron impact ionization involving oxygen dimers 239 (1998) 459
- Krim, L. and M.E. Alikhani, Infrared spectra and theoretical calculations of HCl complexed with NO 237 (1998) 265
- Kück, S. and S. Hartung, Comparative study of the spectroscopic properties of Cr⁴⁺-doped LiAlO₂ and LiGaO₂ 240 (1999) 387
- Kühn, O., see Naundorf, H. 240 (1999) 163
- Kühne, T., R. Küster and P. Vöhringer, Femtosecond photodissociation of triiodide in solution: Excitation energy dependence and transition state dynamics 233 (1998) 161
- Kula, J., M. Kostur and J. Łuczka, Brownian transport controlled by dichotomic and thermal fluctuations 235 (1998) 27
- Kumar, S., see Clarke, N.J. 233 (1998) 9
- Kumar, S., see Bodo, E. 237 (1998) 315
- Kummer, A.D., C. Kompa, H. Lossau, F. Pöllinger-Dammer, M.E. Michel-Beyerle, C.M. Silva, E.J. Bylina, W.J. Coleman, M.M. Yang and D.C. Youvan, Dramatic reduction in fluorescence quantum yield in mutants of Green Fluorescent Protein due to fast internal conversion 237 (1998) 183
- Kuntz, P.J., Diatomics-in-molecules applied to solid hydrogen doped with O(¹D_g) 240 (1999) 19
- Kuo, Y.-C. and J.-P. Hsu, Electrical properties of a charged surface in a general electrolyte solution 236 (1998) 1
- Kurakata, T., see Sato, K. 237 (1998) 195
- Kurtz, H.A., see Cundari, T.R. 240 (1999) 205
- Küster, R., see Kühne, T. 233 (1998) 161
- Kustova, E.V. and E.A. Nagnibeda, Transport properties of a reacting gas mixture with strong vibrational and chemical nonequilibrium 233 (1998) 57
- Lablanquie, P., see Hochlaf, M. 234 (1998) 249
- Ladik, J., see Bogár, F. 237 (1998) 273
- Lai, A., see Marincola, F.C. 236 (1998) 301

- Lane, E., see Castillejo, M. 232 (1998) 353
- Lang, M.J., see Tokmakoff, A. 233 (1998) 231
- Langford, S.R., P.M. Regan, A.J. Orr-Ewing and M.N.R. Ashfold, On the UV photodissociation dynamics of hydrogen iodide 231 (1998) 245
- Langhoff, S.R., see Bauschlicher, Jr., C.W. 234 (1998) 79
- Larkin, A.I., see Feigel'man, M.V. 235 (1998) 107
- Larsson, S., Electronic structure of planar superconducting systems. From finite to extended model 236 (1998) 133
- Lawley, K.P., see Yench, A.J. 238 (1998) 133
- Leach, S., see Bini, R. 232 (1998) 75
- Le Calvé, J., see Uridat, D. 239 (1998) 151
- Lee, Y.T., see Blank, D.A. 231 (1998) 261
- Leigh, D.A., see Brouwer, A.M. 238 (1998) 421
- Lemaire, Ph., see Lembarki, A. 232 (1998) 343
- Lembarki, A., C. Barbier, Ph. Lemaire and E.N. Svendsen, Ab initio variational calculation of dynamic polarizabilities and hyperpolarizabilities. I. Polarizability and quadratic hyperpolarizability of water, carbon monoxide and hydrogen fluoride 232 (1998) 343
- Lemoine, D. and T. Duhoo, Quantum study of oriented NO scattering from Ag(111): orientational steering and effects of surface corrugation 238 (1998) 59
- Leone, S.R., see Frost, M.J. 231 (1998) 145
- Le Sech, C. and B. Silvi, Study of positronium hydride with a simple wavefunction: Application to the Stark effect of PsH 236 (1998) 77
- Leyh, B., see Locht, R. 233 (1998) 145
- Li, F.M., see Chen, J.H. 238 (1998) 165
- Li, G.-S., M.T.C. Martins Costa, C. Millot and M.F. Ruiz-López, Effect of solvent fluctuations on proton transfer dynamics: a hybrid AM1/MM molecular dynamics simulation on the $[H_3N-H-NH_3]^+$ system 240 (1999) 93
- Li, X., see Alexander, M.H. 231 (1998) 331
- Lichanot, A., see Tappero, R. 236 (1998) 97
- Lin, M.C., see Chakraborty, D. 231 (1998) 39
- Lin, S.H., see Berezhkovskii, A.M. 235 (1998) 201
- Lincoln, P., see Marincola, F.C. 236 (1998) 301
- Lindinger, A., see Hartmann, M. 239 (1998) 139
- Lindner, J., K. Ermisch and R. Wilhelm, Multi-photon dissociation of $CHBr_3$ at 248 and 193 nm: observation of the electronically excited $CH(A^2\Delta)$ product 238 (1998) 329
- Line, C.M.B. and G.J. Kearley, The librational and vibrational spectra of water in natrolite, $Na_2Al_2Si_3O_{10} \cdot 2H_2O$ compared with ab-initio calculations 234 (1998) 207
- Linkwitz, S., see Turlot, E. 235 (1998) 47
- Lisek, I., see Kapala, J. 238 (1998) 221
- Lisy, J.M., see Weinheimer, C.J. 239 (1998) 357
- Liu, B.-T., see Hsu, J.-P. 236 (1998) 63
- Liyanage, R., see Alexander, M.H. 231 (1998) 331
- Lloyd, L.D. and R.L. Johnston, Modelling aluminium clusters with an empirical many-body potential 236 (1998) 107
- Lobo, R.F.M., A.M.C. Moutinho and M.J. Calhorda, Fragmentation pathways in the dissociation of fluoro-iodo-benzene negative ions 234 (1998) 265
- Lochbrunner, S., see Fuß, W. 232 (1998) 161

- Locht, R., B. Leyh, K. Hottmann and H. Baumgärtel, A He(I) photoelectron spectroscopic study of the $\tilde{X}^2A''_2$ state of NH_3^+ and ND_3^+ . A reanalysis and evidence for the coriolis coupling between the bending ν_2 and ν_4 modes 233 (1998) 145
- Lommatzsch, U. and B. Brutschy, Ab initio calculations and supersonic jet studies on the geometry of 4-dimethylaminobenzonitrile (DMABN) and related compounds in the ground and excited state 234 (1998) 35
- Lommatzsch, U., see Barth, H.-D. 239 (1998) 49
- Long, X., see Qureshi, F.M. 231 (1998) 87
- Longen, A., see Engemann, C. 237 (1998) 471
- Longo, S. and I.D. Boyd, Nonequilibrium dissociation of hydrogen in a parallel-plate radio frequency discharge 238 (1998) 445
- López, J.C., see Melandri, S. 239 (1998) 229
- López Arbeloa, F., T. López Arbeloa, I. López Arbeloa, I. García-Moreno, A. Costela, R. Sastre and F. Amat-Guerri, Photophysical and lasing properties of pyrromethene 567 dye in liquid solution. Environment effects 236 (1998) 331
- López Arbeloa, I., see López Arbeloa, F. 236 (1998) 331
- López Arbeloa, T., see López Arbeloa, F. 236 (1998) 331
- Lossau, H., see Kummer, A.D. 237 (1998) 183
- Lou, N.-Q., see Wang, M.-L. 238 (1998) 481
- Lounis, B., see Walla, P.J. 233 (1998) 117
- Loureiro, J. and J. Amorim, Dependence of volume-produced H^- ions on the wall recombination probability of H atoms in a low pressure H_2 positive column 232 (1998) 141
- Lu, Z., see Deng, H. 231 (1998) 95
- Łuczka, J., see Kula, J. 235 (1998) 27
- Lufaso, M.W. and A.B. McCoy, Effects of complex formation on reactions of oxygen with HCl and Ar-HCl 239 (1998) 187
- Lunell, S., see Salhi-Benachenhrou, N. 236 (1998) 53
- Luo, Y., see Magnuson, M. 237 (1998) 295
- Luque, F.J., see Colominas, C. 240 (1999) 253
- MacDonald, M.A., see Rennie, E.E. 236 (1998) 365
- MacDonald, M.A., see Baltzer, P. 237 (1998) 451
- Magin, E.H., see Visser, S.A. 240 (1999) 197
- Magnuson, M., L. Yang, J.-H. Guo, C. Sâthe, A. Agui, J. Nordgren, Y. Luo, H. Ågren, N. Johansson, W.R. Salaneck, L.E. Horsburgh and A.P. Monkman, The electronic structure of poly(pyridine-2,5-diyl) investigated by soft X-ray absorption and emission spectroscopies 237 (1998) 295
- Mao, H., see Deng, H. 231 (1998) 95
- Marchesoni, F., see Cattuto, C. 235 (1998) 51
- Marincola, F.C., M. Casu, G. Saba, A. Lai, P. Lincoln and B. Nordén, Recognition and characterization of binding modes of Δ - and Λ -[Ru(phen) $_3$] $^{2+}$ and Δ - and Λ -[Ru(phen) $_2$ DPPZ] $^{2+}$ by the ^{23}Na NMR relaxation and binding free energy parameters 236 (1998) 301
- Märk, T.D., see Muigg, D. 239 (1998) 409
- Marković, N., see Svedung, H. 236 (1998) 189
- Maron, L. and C. Teichtel, On the accuracy of averaged relativistic shape-consistent pseudopotentials 237 (1998) 105
- Marston, G., see Gingell, J.M. 237 (1998) 443
- Martin, J.-L., see Vos, M.H. 233 (1998) 179

- Martin, M., see Castillejo, M. 232 (1998) 353
- Martin, S.J., see Qureshi, F.M. 231 (1998) 87
- Martins, R.F., see Jorge, F.E. 233 (1998) 1
- Martins Costa, M.T.C., see Li, G.-S. 240 (1999) 93
- Martrenchard, S., C. Dedonder-Lardeux, I. Dimicoli, G. Grégoire, C. Jouvet, M. Mons and D. Solgadi, Reactivity of vinyl chloride ionic clusters 239 (1998) 331
- Maslen, P.E., see Faeder, J. 239 (1998) 525
- Mason, N.J., see Gingell, J.M. 237 (1998) 443
- Mataga, N., see Tanaka, F. 236 (1998) 277
- Matsui, A.H., see Takeshima, M. 233 (1998) 97
- Matsui, A.H., see Takeshima, M. 240 (1999) 413
- Matsumi, Y., see Takahashi, K. 231 (1998) 171
- Mayoral, J.A., see Alvira, E. 240 (1999) 101
- McCarroll, R., see Honvault, P. 238 (1998) 401
- McCoy, A.B., see Lufaso, M.W. 239 (1998) 187
- McKee, M.L., see Piety, C.A. 231 (1998) 155
- McKellar, A.J., D. Heryadi, D.L. Yeager and J.A. Nichols, Complete basis set limit ionization potentials of O₃ and NO₂ using the multiconfigurational spin tensor electron propagator method (MCSTEP) 238 (1998) 1
- McKendrick, K.G., see Jackson, N.A. 233 (1998) 45
- McQuaid, M.J. and J.L. Gole, Effect of Al(CO)_x complexation on the aluminum oxidation process 234 (1998) 297
- Melandri, S., J.C. López, P.G. Favero, W. Caminati and J.L. Alonso, Rotational spectrum and dynamics of tetrahydrofuran-argon 239 (1998) 229
- Melinger, J.S., see Kleiman, V.D. 233 (1998) 207
- Meng, Q., see Xiao, C. 237 (1998) 73
- Mennucci, B., see Champagne, B. 238 (1998) 153
- Menzel, C., R. Baumfalk and H. Zacharias, Angular and velocity distributions of small cluster fragments in neutral (NH₃)_n scattering off LiF(100) 239 (1998) 287
- Meyer zum Büschenfelde, D. and A. Staib, Vibrational spectroscopy and molecular dynamics of solvated methanol tetramer and pentamer 236 (1998) 253
- Michel-Beyerle, M.-E., see Voityuk, A.A. 231 (1998) 13
- Michel-Beyerle, M.E., see Kummer, A.D. 237 (1998) 183
- Mikami, N., see Ebata, T. 231 (1998) 199
- Miller, M., see Kapala, J. 238 (1998) 221
- Miller, R.E., see Oudejans, L. 239 (1998) 345
- Millié, P., see Uridat, D. 239 (1998) 151
- Millot, C., see Li, G.-S. 240 (1999) 93
- Minaev, B., see Engström, M. 237 (1998) 149
- Mishra, P.C., see Shukla, M.K. 240 (1999) 319
- Misra, S.K., S. Isber, J.A. Capobianco and E. Cavalli, Electron paramagnetic resonance of Er³⁺ doped in YVO₄: hyperfine parameters 240 (1999) 313
- Mo, Y., see Xiao, C. 237 (1998) 73
- Mohammad-Pooran, S., see Huisken, F. 239 (1998) 11
- Møller, C.K., see Sauer, S.P.A. 238 (1998) 385
- Momicchioli, F., see Baraldi, I. 238 (1998) 353
- Monkman, A.P., see Magnuson, M. 237 (1998) 295
- Monnerville, M., see Pouilly, B. 238 (1998) 437

- Mons, M., see Uridat, D. 239 (1998) 151
Mons, M., see Martrenchard, S. 239 (1998) 331
Morelli, J. and D.J. Tannor, Phase space distribution function approach to the Kramers problem. III. Anharmonic potentials 235 (1998) 213
Morihashi, K., see Yagi, T. 232 (1998) 1
Moriyama, M., Y. Kawakami, S. Tobita and H. Shizuka, Intramolecular proton-transfer cycle of 2,4-dimethoxy-6-(1-hydroxy-2-naphthyl)-s-triazine studied by laser photolysis 231 (1998) 205
Moro, G.J. and F. Cardin, Saddle point avoidance due to inhomogeneous friction 235 (1998) 189
Moutinho, A.M.C., see Lobo, R.F.M. 234 (1998) 265
Muigg, D., G. Denifl, A. Stamatovic, O. Echt and T.D. Märk, High-resolution electron ionization study of CO, (CO)₂ and (CO)₃: appearance energies and bond dissociation energies 239 (1998) 409
Müller, A.M., see Fuß, W. 232 (1998) 161
Müller, B.G., see Hu, Z. 232 (1998) 63
Müller, J., D. Haarer, O.V. Khodykin and B.M. Kharlamov, Investigation of spectral diffusion in PMMA on timescales from 10⁻⁵ to 10⁴ seconds via transient and photophysical hole burning 237 (1998) 483
Müller-Dethlefs, K., see Chapman, D.M. 239 (1998) 417
Munn, R.W., Role of the local electric field in electro-absorption spectra of molecular crystals 236 (1998) 151
Murai, H., see Kitahama, Y. 238 (1998) 429
Murphy, A., see Brouwer, A.M. 238 (1998) 421

Nagao, K., see Ebata, T. 231 (1998) 199
Nagnibeda, E.A., see Kustova, E.V. 233 (1998) 57
Nakabayashi, T., see Okamoto, H. 236 (1998) 309
Nakai, Y., see Ohashi, K. 239 (1998) 429
Nakane, Y., see Ohashi, K. 239 (1998) 429
Nardi, F., see Knapp-Mohammady, M. 240 (1999) 63
Naumkin, F.Y., DIM models for RgX₂⁻ systems: suppressed influence of spin-orbit coupling and induced multipole effects for the Ar-I₂⁻ interaction 240 (1999) 79
Naundorf, H., K. Sundermann and O. Kühn, Laser driven hydrogen tunneling in a dissipative environment 240 (1999) 163
Neidlinger, T., see Barvík, I. 240 (1999) 173
Nemukhin, A.V., see Grigorenko, B.L. 232 (1998) 321
Nesbitt, D.J., see Anderson, D.T. 239 (1998) 253
Nešpůrek, S., see Kadashchuk, A. 234 (1998) 285
Nešpůrek, S., see Sworakowski, J. 238 (1998) 343
Neumann, R., see Zuhrt, C. 240 (1999) 117
Neumark, D.M., see Schiedt, J. 239 (1998) 511
Neusser, H.J., see Helm, R.M. 239 (1998) 33
Neville, J.J., A. Jürgensen, R.G. Cavell, N. Kosugi and A.P. Hitchcock, Inner-shell excitation of PF₃, PCl₃, PCl₂CF₃, OPF₃ and SPF₃. Part I. Spectroscopy 238 (1998) 201
Newton, M.D., M.V. Basilevsky and I.V. Rostov, A frequency-resolved cavity model (FRCM) for treating equilibrium and non-equilibrium solvation energies. 2: Evaluation of solvent reorganization energies 232 (1998) 201
Newton, M.D., see Basilevsky, M.V. 232 (1998) 189
Ng, C.Y., see Hsu, C.-W. 231 (1998) 121

- Nguyen, M.T., see Chandra, A.K. 232 (1998) 299
- Nichols, J.A., see McKellar, A.J. 238 (1998) 1
- Nickel, B. and P.J. Walla, Peculiarity of triplet–triplet energy transfer from 2-(2'-hydroxy-phenyl)benzoxazole to diacetyl. Evidence for radiative keto–enol transitions $^3K^* \rightarrow ^1E$ and $^1E \rightarrow ^1K^*$ 237 (1998) 371
- Nicovich, J.M., see Piety, C.A. 231 (1998) 155
- Niedner-Schatteburg, G., see Berg, C. 239 (1998) 379
- Nieuwpoort, W.C., see de Graaf, C. 237 (1998) 59
- Nishi, N., see Ohashi, K. 239 (1998) 429
- Nishimura, Y., see Tsuji, M. 236 (1998) 319
- Nitzan, A., see Graf, P. 235 (1998) 297
- Nizkorodov, S.A. and E.J. Bieske, Photofragmentation dynamics of the $(N_2O)_2^+$ and $(N_2O)_3^+$ clusters: fragment N_2O^+ A \leftarrow X spectra 239 (1998) 369
- Nizkorodov, S.A., see Olkhov, R.V. 239 (1998) 393
- Nordén, B., see Marincola, F.C. 236 (1998) 301
- Nordgren, J., see Magnuson, M. 237 (1998) 295
- Nordholm, S., see Svedung, H. 236 (1998) 189
- Nordio, P.L., see Bordes, B. 231 (1998) 51
- Nordio, P.L., see Polimeno, A. 235 (1998) 313
- Obi, K., see Tsuji, K. 231 (1998) 279
- Oda, E., see Tsuji, M. 236 (1998) 319
- Ogura, M., see Okamoto, H. 236 (1998) 309
- Ohashi, K., Y. Nakane, Y. Inokuchi, Y. Nakai and N. Nishi, Photodissociation spectroscopy of (benzene–toluene) $^+$. Charge delocalization in the hetero-dimer ion 239 (1998) 429
- Okamoto, H., M. Ogura, T. Nakabayashi and M. Tasumi, Sub-picosecond excited-state dynamics of a carotenoid (spirilloxanthin) in the light-harvesting systems of *Chromatium vinosum*. Relaxation process from the optically allowed S_2 state 236 (1998) 309
- Okunuki, Y., see Zils, R. 231 (1998) 303
- Olkhov, R.V., S.A. Nizkorodov and O. Dopfer, Infrared photodissociation spectra of isomeric $SiOH^+-Ar_n$ ($n = 1-10$) complexes 239 (1998) 393
- Olney, T.N., G. Cooper and C.E. Brion, Quantitative studies of the photoabsorption (4.5–488 eV) and photoionization (9–59.5 eV) of methyl iodide using dipole electron impact techniques 232 (1998) 211
- Olson, J.A., see Guan, D. 233 (1998) 35
- Oppel, M. and G.K. Paramonov, Ultrafast laser control of vibrational dynamics for a two-dimensional model of $HONO_2$ in the ground electronic state: separation of conformers, control of the bond length, selective preparation of the discrete and the continuum states 232 (1998) 111
- Ordonez, C.A., see Chang, Y. 231 (1998) 27
- Orea, J.M., see Garay, M. 236 (1998) 343
- Orlandi, G., see Bini, R. 232 (1998) 75
- Ornellas, F.R. and S. Iwata, A theoretical study of the electronic structure and spectroscopic properties of the low-lying electronic states of the molecule $AlSi$ 232 (1998) 95
- Orozco, M., see Colominas, C. 240 (1999) 253
- Orr-Ewing, A.J., see Langford, S.R. 231 (1998) 245
- Orrit, M., see Walla, P.J. 233 (1998) 117
- Ortica, F., see Romani, A. 237 (1998) 413

- Orzechowski, K., Electric field effect on the upper critical solution temperature 240 (1999) 275
- Ostapenko, N., see Kadashchuk, A. 234 (1998) 285
- Ostojić, B., see Perić, M. 231 (1998) 105
- Ostrovsky, S.M., see Borrás-Almenar, J.J. 240 (1999) 149
- Oudejans, L. and R.E. Miller, Mode dependence of the state-to-state vibrational dynamics of HCN–HF 239 (1998) 345
- Ovchinnikov, A.A. and K.A. Pronin, Field-induced localization and nonlinear response of a one-band conductor to a periodic electric field 235 (1998) 93
- Paidarová, I., see Sauer, S.P.A. 238 (1998) 385
- Pal, H., see Shirota, H. 236 (1998) 355
- Palii, A.V., see Borrás-Almenar, J.J. 240 (1999) 149
- Palmer, M.H., I.C. Walker and M.F. Guest, The electronic states of pyrrole studied by optical (VUV) absorption, near-threshold electron energy-loss (EEL) spectroscopy and ab initio multi-reference configuration interaction calculations 238 (1998) 179
- Palmer, P.M. and M.R. Topp, Electronic spectroscopy of jet-cooled anthracene/(H₂O)_n clusters (*n* = 1–16): comparisons of inhomogeneous structure 239 (1998) 65
- Papp, G., see Gudowska-Nowak, E. 232 (1998) 247
- Paramonov, G.K., see Oppel, M. 232 (1998) 111
- Park, J., see Chakraborty, D. 231 (1998) 39
- Parker, A.W., see Scholes, G.D. 234 (1998) 21
- Parker, J.E., see Rennie, E.E. 236 (1998) 365
- Parneix, P., F.G. Amar and P. Bréchnignac, On the use of evaporation dynamics to characterize phase transitions in van der Waals clusters: investigations in aniline–(argon)_n up to *n* = 15 239 (1998) 121
- Parry, D.E., see Griffiths, I.W. 238 (1998) 21
- Parson, R., see Faeder, J. 239 (1998) 525
- Parusel, A.B.J., see Welland, A.D. 240 (1999) 403
- Pasquarello, A., see Jimenez, S. 233 (1998) 343
- Paterlini, M.G. and D.M. Ferguson, Constant temperature simulations using the Langevin equation with velocity Verlet integration 236 (1998) 243
- Pauls, S.W., J.F. Hedstrom and C.K. Johnson, Rotational relaxation of perylene in *n*-alcohols and *n*-alkanes studied by two-photon-induced anisotropy decay 237 (1998) 205
- Pawlikowski, M., see Andruniow, T. 236 (1998) 25
- Pawlikowski, M., see Andruniow, T. 236 (1998) 35
- Pechukas, P. and J. Ankerhold, Mathematical aspects of the fluctuating barrier problem. Existence of equilibrium and relaxation solutions 235 (1998) 5
- Pecul, M. and J. Sadlej, Solvent effects on NMR spectrum of acetylene calculated by ab initio methods 234 (1998) 111
- Pedulla, J.M. and K.D. Jordan, Melting behavior of the (H₂O)₆ and (H₂O)₈ clusters 239 (1998) 593
- Penent, F., see Hochlaf, M. 234 (1998) 249
- Perić, M., B. Ostojić, B. Schäfer and B. Engels, Erratum to “*Ab initio* treatment of the Renner-Teller effect in tetra-atomic molecules undergoing large amplitude bending vibrations” [Chem. Phys. 225 (1997) 63–76] 231 (1998) 105
- Perić, M., B. Engels and M. Hanrath, Ab initio study of the electronic spectrum of C₂H₂⁺. I. Vertical spectrum and angular potential curves 238 (1998) 33
- Perić, M. and B. Engels, Ab initio study of the electronic spectrum of C₂H₂⁺. II. Stretching potential energy surfaces for low-lying doublet electronic states 238 (1998) 47

- Peřina, Jr., J., Interplay of creation, propagation, and relaxation of an excitation in a dimer 236 (1998) 157
- P  riquet, V., see Desfr  n  is, C. 239 (1998) 475
- Petelenz, P., see Eilmes, A. 237 (1998) 67
- Petrella, G., L. Cassidei and F. Ciriaco, The correlation between the statistical properties of surface defect distribution and the specular intensity obtained from low energy He scattering technique 231 (1998) 31
- Pettinger, B., see Beltramo, G. 238 (1998) 473
- Phillips, D., see Scholes, G.D. 234 (1998) 21
- Philpott, M.J., S.C. Hayes and P.J. Reid, Femtosecond pump-probe studies of chlorine dioxide photochemistry in water and acetonitrile 236 (1998) 207
- Piety, C.A., R. Soller, J.M. Nicovich, M.L. McKee and P.H. Wine, Kinetic and mechanistic study of the reaction of atomic chlorine with methyl bromide over an extended temperature range 231 (1998) 155
- Pilling, M.J., see Gang, J. 231 (1998) 183
- Pinot de Moira, J.C., see Denzer, W. 231 (1998) 109
- Piuzzi, F., see Uridat, D. 239 (1998) 151
- Plashkevych, O., V. Carravetta, O. Vahtras and H.   gren, Theoretical study of X-ray circular dichroism of amino acids 232 (1998) 49
- Poizat, O., see Didierjean, C. 237 (1998) 169
- Pol  k, R., Bonding in molecular dications from the classical valence bond viewpoint. A case study of CO²⁺ 232 (1998) 25
- Polavarapu, P.L. and D.K. Chakraborty, Ab initio theoretical optical rotations of small molecules 240 (1999) 1
- Polimeno, A., G. Saielli and P.L. Nordio, A diffusive model for interpreting solvation dynamics in isotropic and ordered liquid phases 235 (1998) 313
- Pollak, E., see Talkner, P. 235 (1998) 131
- P  llinger-Dammer, F., see Kummer, A.D. 237 (1998) 183
- Polster, J., Contributions to the spectroscopic-kinetic analysis of linear reaction systems. Systems with three linearly independent reactions using the concept of parallel projection 240 (1999) 331
- Pongor, G., see Kov  cs, A. 238 (1998) 231
- Ponterini, G., see Baraldi, I. 238 (1998) 353
- Popari  , G., M. Vi  i   and D.S. Beli  , Vibrational excitation of the C³  _u state of N₂ by electron impact 240 (1999) 283
- Porcher, P., see Cascales, C. 240 (1999) 291
- Poth, L., Q. Zhong, J.V. Ford, S.M. Hurley and A.W. Castleman Jr., Charge stripping effects from highly charged iodine ions formed from Coulomb explosion of CH₃I clusters 239 (1998) 309
- Pouilly, B. and M. Monnerville, New investigation of the photodissociation of the HBr molecule: total cross-section, anisotropy parameter and dependence of the spin-orbit branching on the ground state vibrational level 238 (1998) 437
- Pronin, K.A., see Ovchinnikov, A.A. 235 (1998) 93
- Pshenichnikov, M.S., see de Boeij, W.P. 233 (1998) 287
- Pullins, S.H., see France, M.R. 239 (1998) 447
- Pykhov, R.L., see Sharafutdinov, R.G. 233 (1998) 127
- Qureshi, F.M., S.J. Martin, X. Long, D.D.C. Bradley, F.Z. Henari, W.J. Blau, E.C. Smith, C.H. Wang, A.K. Kar and H.L. Anderson, Optical limiting properties of a zinc porphyrin polymer and its dimer and monomer model compounds 231 (1998) 87

- Rabinovitz, M., see Beust, R. 240 (1999) 141
- Raimondi, M., see Famulari, A. 232 (1998) 275
- Raimondi, M., see Famulari, A. 232 (1998) 289
- Raimondi, M., see Clarke, N.J. 233 (1998) 9
- Raimondi, M., see Bodo, E. 237 (1998) 315
- Randall, C.J., see Jackson, N.A. 233 (1998) 45
- Ravishankara, A.R., see Gierczak, T. 231 (1998) 229
- Reese, S.K. and S.C. Tucker, Curvilinear-path based theory of the energy transfer limited rate of a two-dimensional solute in a dissipative bath 235 (1998) 171
- Regan, P.M., see Langford, S.R. 231 (1998) 245
- Reid, P.J., see Philpott, M.J. 236 (1998) 207
- Reimann, B., see Barth, H.-D. 239 (1998) 49
- Reimann, P., R. Bartussek and P. Hänggi, Reaction rates when barriers fluctuate: A singular perturbation approach 235 (1998) 11
- Reimann, P., see Thorwart, M. 235 (1998) 61
- Reineker, P., see Barvík, I. 240 (1999) 173
- Reinen, D., see Hu, Z. 232 (1998) 63
- Rennie, E.E., C.A.F. Johnson, J.E. Parker, D.M.P. Holland, D.A. Shaw, M.A. MacDonald, M.A. Hayes and L.G. Shpinkova, A study of the spectroscopic and thermodynamic properties of furan by means of photoabsorption, photoelectron and photoion spectroscopy 236 (1998) 365
- Requena, A., see Bastida, A. 240 (1999) 229
- Resende, S.M. and W.B. De Almeida, Analysis of the reaction paths to dissociation of dichloro-ethylenes into Cl_2 and C_2H_2 238 (1998) 11
- Rinaldi, C.A., see Garay, M. 236 (1998) 343
- Ríos, M.A., see Cabaleiro-Lago, E.M. 236 (1998) 235
- Rips, I., Nonadiabatic reactions in condensed phase in the absence of thermal equilibrium 235 (1998) 243
- Robertson, S.H., see Gang, J. 231 (1998) 183
- Robinson, G.W., see Cho, C.H. 232 (1998) 329
- Romani, A., F. Ortica and G. Favaro, Proximity effects in the excited state ordering and photophysics of thienyl-pyridyl ketones 237 (1998) 413
- Roncero, O., see Janda, K.C. 239 (1998) 177
- Rösch, N., see Voityuk, A.A. 231 (1998) 13
- Rostov, I.V., see Basilevsky, M.V. 232 (1998) 189
- Rostov, I.V., see Newton, M.D. 232 (1998) 201
- Roszak, S., see Kapala, J. 238 (1998) 221
- Roth, W., M. Schmitt, Ch. Jacoby, D. Spangenberg, Ch. Janzen and K. Kleinermmanns, Double resonance spectroscopy of phenol(H_2O)₁₋₁₂: evidence for ice-like structures in aromate-water clusters? 239 (1998) 1
- Roth, W., see Jacoby, C. 239 (1998) 23
- Rüchardt, Ch., see Bini, R. 232 (1998) 75
- Rudolf, P., see Brouwer, A.M. 238 (1998) 421
- Ruf, M.-W., see Weber, J.M. 239 (1998) 271
- Ruf, M.-W., see Kreil, J. 239 (1998) 459
- Ruiz, J., see Castillejo, M. 232 (1998) 353
- Ruiz-López, M.F., see Li, G.-S. 240 (1999) 93
- Rurali, R., see Consolati, G. 237 (1998) 493
- Rusin, L.Yu., see Azriel, V.M. 232 (1998) 307

- Rutkowski, K.S., IR–IR double-resonance studies of vibrational relaxation of CD₃F in solid and liquid Xe, Kr, Ar solutions near the melting point 237 (1998) 403
- Saba, G., see Marincola, F.C. 236 (1998) 301
- Sadeghi, R., see Skodje, R.T. 240 (1999) 129
- Sadlej, J., see Pecul, M. 234 (1998) 111
- Sáez Puche, R., see Cascales, C. 240 (1999) 291
- Saielli, G., see Polimeno, A. 235 (1998) 313
- Saito, N., see Suzuki, I.H. 234 (1998) 255
- Sakimoto, K., A semiclassical study of dissociation dynamics in He + H₂ collisions 236 (1998) 123
- Salaneck, W.R., see Magnuson, M. 237 (1998) 295
- Salhi-Benachenhou, N., B. Engels, M.-B. Huang and S. Lunell, Theoretical study of the ethylene radical cation: geometry and hyperfine structure 236 (1998) 53
- Sandall, J.P.B., see Bini, R. 232 (1998) 75
- Sastre, R., see López Arbeloa, F. 236 (1998) 331
- Sastre, R., see Barroso, J. 238 (1998) 257
- Såthe, C., see Magnuson, M. 237 (1998) 295
- Sato, K., N. Ishida, T. Kurakata, A. Iwasaki and S. Tsunashima, Reactions of C(¹D) with H₂, HD and D₂: kinetic isotope effect and the CD/CH branching ratio 237 (1998) 195
- Sato, S., see Tanaka, D. 239 (1998) 437
- Sauer, S.P.A., C.K. Møller, H. Koch, I. Paidarová and V. Špirko, The vibrational and temperature dependence of the indirect nuclear spin–spin coupling constants of the oxonium (H₃O⁺) and hydroxyl (OH[−]) ions 238 (1998) 385
- Schäfer, B., see Perić, M. 231 (1998) 105
- Schermann, J.P., see Desfrancois, C. 239 (1998) 475
- Schiebel, P., see Detken, A. 238 (1998) 301
- Schiedt, J., R. Weinkauff, D.M. Neumark and E.W. Schlag, Anion spectroscopy of uracil, thymine and the amino-oxo and amino-hydroxy tautomers of cytosine and their water clusters 239 (1998) 511
- Schikarski, T., see Fuß, W. 232 (1998) 161
- Schlag, E.W., see Schiedt, J. 239 (1998) 511
- Schmickler, W., see Beltramo, G. 238 (1998) 473
- Schmid, W.E., see Fuß, W. 232 (1998) 161
- Schmidt, B., see Korolkov, M.V. 237 (1998) 123
- Schmitt, M., see Roth, W. 239 (1998) 1
- Schmitt, M., see Jacoby, C. 239 (1998) 23
- Schneider, F.W., see Welland, A.D. 240 (1999) 403
- Scholes, G.D., I.R. Gould, A.W. Parker and D. Phillips, Time-resolved resonance Raman and molecular orbital studies of charge separation and intramolecular reorganisation 234 (1998) 21
- Schriver, A., see Hallou, A. 237 (1998) 251
- Schriver-Mazzuoli, L., see Hallou, A. 237 (1998) 251
- Schuder, M., see Anderson, D.T. 239 (1998) 253
- Schulze, K.-D., Impedance spectroscopic investigation of the temperature influence on the transfer of tetraphenylborate ions through lipid membranes — Calculation of energy barriers for the ion transfer across lipid membranes 238 (1998) 495
- Schuss, Z. and A. Spivak, Where is the exit point? 235 (1998) 227
- Schütz, M., see Hartke, B. 239 (1998) 561
- Schwentner, N., see Zadoyan, R. 233 (1998) 353

- Seel, M., see Wolfseder, B. 233 (1998) 323
- Seidner, L., see Wolfseder, B. 233 (1998) 323
- Seilmeier, A., see Dahinten, T. 232 (1998) 239
- Seliger, J., ^{17}O quadrupole coupling in $\text{C}-\text{O}-\text{H} \cdots \text{O}=\text{C}$ hydrogen bonds 231 (1998) 81
- Seliger, J. and V. Žagar, ^{17}O nuclear quadrupole resonance study of proton disorder in solid benzoic acid, 4-hydroxybenzoic acid and 4-nitrobenzoic acid 234 (1998) 223
- Senapati, S. and A. Chandra, Molecular relaxation in simple dipolar liquids confined between two solid surfaces 231 (1998) 65
- Sevryuk, M.B., see Azriel, V.M. 232 (1998) 307
- Shao, J., C. Zerbe and P. Hänggi, Suppression of quantum coherence: Noise effect 235 (1998) 81
- Sharafutdinov, R.G., A.A. Ilyukhin, V.V. Smirnov, A.E. Belikov, G.I. Sukhinin and R.L. Pykhov, Populations of rotational levels of nitrogen molecules in free jets. Comparison of CARS and electron beam fluorescent technique 233 (1998) 127
- Shaw, D.A., see Rennie, E.E. 236 (1998) 365
- Shchepkin, D.N., see Kolomiitsova, T.D. 238 (1998) 315
- Shen, Y., see Deng, H. 231 (1998) 95
- Shen, Z.W., see Yan, Y.J. 233 (1998) 191
- Shibuya, K., see Tsuji, K. 231 (1998) 279
- Shimono, A., see Takami, A. 231 (1998) 215
- Shirota, H., H. Pal, K. Tominaga and K. Yoshihara, Ultrafast intermolecular electron transfer in coumarin-hydrazine system 236 (1998) 355
- Shirota, H., N. Endo and K. Horie, Volume phase transition of polymer gel in water and heavy water 238 (1998) 487
- Shizuka, H., see Moriyama, M. 231 (1998) 205
- Shpinkova, L.G., see Rennie, E.E. 236 (1998) 365
- Shukla, M.K. and P.C. Mishra, A gas phase ab initio excited state geometry optimization study of thymine, cytosine and uracil 240 (1999) 319
- Shushin, A.I. and M. Tachiya, Non-adiabatic effects in condensed phase activated rate processes in the near-adiabatic limit 235 (1998) 267
- Siebbeles, L.D.A. and Y.A. Berlin, Quantum motion of particles along one-dimensional pathways with static and dynamic energy disorder 238 (1998) 97
- Siebers, J.G., U. Buck and T.A. Beu, Calculation of structures and vibrational spectra of acetonitrile clusters 239 (1998) 549
- Siggel, M.R.F., see Gingell, J.M. 237 (1998) 443
- Silva, C.M., see Kummer, A.D. 237 (1998) 183
- Silvi, B., see Le Sech, C. 236 (1998) 77
- Singh, J., see Takeshima, M. 233 (1998) 97
- Singh, S., see Cho, C.H. 232 (1998) 329
- Sironi, M., see Famulari, A. 232 (1998) 275
- Sironi, M., see Famulari, A. 232 (1998) 289
- Sironi, M., see Clarke, N.J. 233 (1998) 9
- Sironi, M., see Bodo, E. 237 (1998) 315
- Sivachenko, A.Yu., see Burshtein, A.I. 235 (1998) 257
- Skinner, J.L., see Everitt, K.F. 235 (1998) 115
- Skodje, R.T., R. Sadeghi and J.L. Krause, Control of transition state spectra: a variational algorithm 240 (1999) 129
- Smirnov, K.S., see Ermoshin, V.A. 237 (1998) 333
- Smirnov, V.V., see Sharafutdinov, R.G. 233 (1998) 127

- Smith, E.C., see Qureshi, F.M. 231 (1998) 87
- Smith, M.A., see Belikov, A.E. 234 (1998) 195
- Sobolewski, A.L. and W. Domcke, *Ab initio* study of excited-state intramolecular proton dislocation in salicylic acid 232 (1998) 257
- Sobolewski, A.L., see Sudholt, W. 240 (1999) 9
- Sokolov, I.M. and A. Blumen, Thermodynamical and mechanical efficiency of a ratchet pump 235 (1998) 39
- Solà, M., see Forés, M. 234 (1998) 1
- Solgadi, D., see Martrenchard, S. 239 (1998) 331
- Soller, R., see Piety, C.A. 231 (1998) 155
- Song, J.-B. and E.A. Gislason, Theoretical study of the effect of reagent rotation and vibration on the reactions of $\text{Cl} + \text{H}_2$ and $\text{Cl} + \text{HD}$ 237 (1998) 159
- Soos, Z.G., see Kiselev, S.A. 238 (1998) 365
- Soudackov, A.V., see Basilevsky, M.V. 235 (1998) 281
- Spadacini, R., see Caratti, G. 235 (1998) 157
- Spangenberg, D., see Roth, W. 239 (1998) 1
- Spanget-Larsen, J., Infrared absorption and Raman scattering of (Z)-3-hydroxypropenal. A density functional theoretical study 240 (1999) 51
- Špirko, V., see Sauer, S.P.A. 238 (1998) 385
- Špirko, V., see Chapman, D.M. 239 (1998) 417
- Spivak, A., see Schuss, Z. 235 (1998) 227
- Spoerel, U. and W. Stahl, Equatorial piperidine and the piperidine–water complex. Rotational spectra and molecular structures 239 (1998) 97
- Spoerel, U. and D. Consalvo, A contribution to the structure determination of Ar–thiophene: the electric dipole moment 239 (1998) 199
- Sprang, H., see Campbell, E.E.B. 239 (1998) 299
- Stahl, W., see Spoerel, U. 239 (1998) 97
- Staib, A., see Meyer zum Büschenfelde, D. 236 (1998) 253
- Stamatovic, A., see Muigg, D. 239 (1998) 409
- Stampor, W., see Kalinowski, J. 237 (1998) 233
- Stefanetti, M., see Consolati, G. 237 (1998) 493
- Steffen, T. and K. Duppen, Population relaxation and non-Markovian frequency fluctuations in third- and fifth-order Raman scattering 233 (1998) 267
- Stener, M., see Fronzoni, G. 232 (1998) 9
- Stener, M., see Venuti, M. 234 (1998) 95
- Stimson, S., see Hsu, C.-W. 231 (1998) 121
- Stock, G., see Wolfseder, B. 233 (1998) 323
- Storm, V., H. Dreizler and D. Consalvo, Rotational spectra of the ^{15}N -aniline–X, (X = Ar, Ne) complexes. Structure determination from studies on isotopomers 237 (1998) 395
- Storm, V., H. Dreizler and D. Consalvo, A contribution to the rotational spectrum, structure, and dynamics of the benzonitrile–water complex in the S_0 electronic state 239 (1998) 109
- Sudholt, W., A.L. Sobolewski and W. Domcke, *Ab initio* study of the amino group twisting and wagging reaction paths in the intramolecular charge transfer of 4-(N,N-dimethyl-amino)benzonitrile 240 (1999) 9
- Suhai, S., see Knapp-Mohammady, M. 240 (1999) 63
- Suits, A.G., see Blank, D.A. 231 (1998) 261
- Sukhinin, G.I., see Sharafutdinov, R.G. 233 (1998) 127
- Sundermann, K., see Naundorf, H. 240 (1999) 163

- Sundström, V., see Fidder, H. 233 (1998) 311
Suto, K., see Fiss, J.A. 233 (1998) 335
Suzuki, I.H. and N. Saito, Fragment ion yields from CFCl_3 photoexcited in regions of the Cl2p, the Cl1s, and the F1s electron transitions 234 (1998) 255
Suzuki, T., see Katayanagi, H. 231 (1998) 345
Svedung, H., L.E.B. Börjesson, N. Marković and S. Nordholm, The mechanism of energy transfer in $\text{H}_2\text{O}-\text{H}_2\text{O}$ collisions – a molecular dynamics simulation 236 (1998) 189
Svendsen, E.N., see Lembarki, A. 232 (1998) 343
Swiatla-Wojcik, D., see Hawlicka, E. 232 (1998) 361
Sworakowski, J. and S. Nešpůrek, 'Fractional heating' differential scanning calorimetry: a tool to study energetics and kinetics of solid-state reactions in photoactive systems with distributed parameters 238 (1998) 343
Szczęśniak, M.M., see Jakowski, J. 239 (1998) 573

Tachiya, M., see Shushin, A.I. 235 (1998) 267
Tadjeddine, M. and J.P. Flament, Analysis of a nonlinear optical response of CN^- ions adsorbed on metal electrode: tentative interpretation by means of ab initio molecular calculations 240 (1999) 39
Takahashi, K., N. Taniguchi, Y. Matsumi and M. Kawasaki, Translational energy and angular distributions of $\text{O}(^1\text{D})$ and $\text{O}(^3\text{P}_j)$ fragments in the UV photodissociation of ozone 231 (1998) 171
Takami, A., S. Kato, A. Shimono and S. Koda, Uptake coefficient of OH radical on aqueous surface 231 (1998) 215
Takase, H., see Yagi, T. 232 (1998) 1
Takeshima, M., J. Singh and A.H. Matsui, Instability of self-trapped Frenkel exciton states in one-dimensional microcrystallites 233 (1998) 97
Takeshima, M. and A.H. Matsui, Frenkel exciton scattering at microcrystallite surfaces caused by electric dipoles and monopoles 240 (1999) 413
Talbi, D. and M.C. Bacchus-Montabonel, Ab-initio study of a radiative association mechanism application to the $\text{CH}_3^+ + \text{H}_2$ reaction 232 (1998) 267
Talkner, P., E. Pollak and A.M. Berezhkovskii, Binary collision theory for thermal and nonisothermal relaxation and reaction of polyatomic molecules 235 (1998) 131
Tamarat, Ph., see Walla, P.J. 233 (1998) 117
Tanaka, D., S. Sato and K. Kimura, ZEKE electron spectroscopy of azulene and azulene-argon 239 (1998) 437
Tanaka, F. and N. Mataga, Analytical theory of time-resolved fluorescence anisotropy and dynamic stokes shift of polar solute molecules based on continuum model for solvent 236 (1998) 277
Tanaka, I., see Kawaguchi, K. 231 (1998) 193
Tanaka, M., see Tsuji, M. 236 (1998) 319
Taniguchi, N., see Takahashi, K. 231 (1998) 171
Tanimura, Y., Fifth-order two-dimensional vibrational spectroscopy of a Morse potential system in condensed phases 233 (1998) 217
Tannor, D.J., see Morelli, J. 235 (1998) 213
Tappero, R. and A. Lichanot, A comparative study of the electronic structure of $\alpha\text{-MnS}$ (alabandite) calculated at the Hartree-Fock and Density Functional levels of theory 236 (1998) 97
Tasumi, M., see Okamoto, H. 236 (1998) 309
Teichteil, C., see Maron, L. 237 (1998) 105
Teixidó, J., see Colominas, C. 240 (1999) 253

- Temme, F.P., Yamanouchi-chain \mathcal{S}_n -invariant hierarchies for SR carrier space of $\{T^k(v)\}(SU2 \times \mathcal{S}_n)$ dual tensors in NMR: some maximal \mathcal{S}_n -inner products, via \mathcal{S}_n -restricted-space Schur Fn. product mappings 238 (1998) 245
- Thiel, S., T. Klüner and H.-J. Freund, Interference-effects in the laser-induced desorption of small molecules from surfaces: a model study 236 (1998) 263
- Thorwart, M., P. Reimann, P. Jung and R.F. Fox, Quantum hysteresis and resonant tunneling in bistable systems 235 (1998) 61
- Tobita, S., see Moriyama, M. 231 (1998) 205
- Toennies, J.P., see Azriel, V.M. 232 (1998) 307
- Toennies, J.P., see Hartmann, M. 239 (1998) 139
- Tokmakoff, A., M.J. Lang, X.J. Jordanides and G.R. Fleming, The intermolecular interaction mechanisms in liquid CS₂ at 295 and 165 K probed with two-dimensional Raman spectroscopy 233 (1998) 231
- Tolkatchev, V.A., see Vyazovkin, V.L. 236 (1998) 291
- Tomasi, J., see Champagne, B. 238 (1998) 153
- Tominaga, K., see Shirota, H. 236 (1998) 355
- Tommei, G.E., see Caratti, G. 235 (1998) 157
- Topp, M.R., see Palmer, P.M. 239 (1998) 65
- Trakhtenberg, L.I. and V.L. Klochikhin, Effect of pressure and temperature on the H-atom tunneling in solid phase chemical reactions. The acridine/fluorene system 232 (1998) 175
- Trommsdorff, H.P., see Benderskii, V.A. 234 (1998) 153
- Trushin, S.A., see Fuß, W. 232 (1998) 161
- Tsai, C.Y., S.P. Chen and T.C. Wen, Nonlinear absorption and refraction in porphyrazine derivatives 240 (1999) 191
- Tsuji, K., K. Aiuchi, K. Shibuya and K. Obi, Electronic spectroscopy and predissociation mechanism of Ar–NO in the 3p Rydberg states 231 (1998) 279
- Tsuji, M., M. Tanaka, E. Oda, H. Ishimi and Y. Nishimura, Emission spectra of HeAr₂⁺ and HeKr₂⁺ heterotrimer ions produced in a helium flowing afterglow 236 (1998) 319
- Tsukerblat, B.S., see Borrás-Almenar, J.J. 240 (1999) 149
- Tsunashima, S., see Sato, K. 237 (1998) 195
- Tucker, S.C., see Reese, S.K. 235 (1998) 171
- Turlot, E., S. Linkwitz, D. Esteve, C. Urbina, M.H. Devoret and H. Grabert, High frequency satellites in resonant activation 235 (1998) 47
- Tyley, P.L., see Denzer, W. 231 (1998) 109
- Tyutyulkov, N., see Beust, R. 240 (1999) 141
- Ulness, D.J., J.C. Kirkwood and A.C. Albrecht, On librational broadening of vibrational transitions in liquids: a simple model 240 (1999) 109
- Urbina, C., see Turlot, E. 235 (1998) 47
- Uridat, D., V. Brenner, I. Dimicoli, J. Le Calvé, P. Millié, M. Mons and F. Piuze, Existence of two internal energy distributions in jet-formed van der Waals heteroclusters: example of the anthracene–argon_n system 239 (1998) 151
- Vahtras, O., see Plashkevych, O. 232 (1998) 49
- Vahtras, O., see Engström, M. 237 (1998) 149
- Vandenbroucke, D., see Gilliams, B. 237 (1998) 91
- Vanossi, D., see Baraldi, I. 238 (1998) 353
- Varandas, A.J.C., see Wang, W. 236 (1998) 181

- Velev, P. and M.F. Herman, A semiclassical surface-hopping procedure for vibrational relaxation in polyatomic molecules: model calculations 240 (1999) 241
- Velino, B., see Caminati, W. 239 (1998) 223
- Vener, M.V., Model study of proton transfer in a H-bonded cluster with an A-H...B reaction complex. Introduction of an effective coordinate for the solvation shell 233 (1998) 77
- Venuti, M., M. Stener and P. Decleva, Valence photoionization of C_6H_6 by the B-spline one-centre expansion density functional method 234 (1998) 95
- Vetoshkin, E.V., see Benderskii, V.A. 234 (1998) 153
- Vetoshkin, E.V., see Benderskii, V.A. 234 (1998) 173
- Vičić, M., see Poparić, G. 240 (1999) 283
- Vilesov, A.F., see Hartmann, M. 239 (1998) 139
- Visser, S.A., W.T. Gruenbaum, E.H. Magin and P.M. Borsenberger, Hole transport in arylamine doped polymers 240 (1999) 197
- Vöhringer, P., see Kühne, T. 233 (1998) 161
- Voityuk, A.A., M.-E. Michel-Beyerle and N. Rösch, Quantum chemical modeling of structure and absorption spectra of the chromophore in green fluorescent proteins 231 (1998) 13
- Voronin, A.I., see Basilevsky, M.V. 235 (1998) 281
- Vos, M.H., M.R. Jones and J.-L. Martin, Vibrational coherence in bacterial reaction centers: spectroscopic characterisation of motions active during primary electron transfer 233 (1998) 179
- Voth, G.A., see Hernandez, R. 233 (1998) 243
- Vyazovkin, V.L. and V.A. Tolkatchev, Isotope effect in diffusion of methyl radicals in glassy ethanol-1,2- d_5 at low temperatures 236 (1998) 291
- Wade, R.C., see Knapp-Mohammady, M. 240 (1999) 63
- Walker, I.C., see Palmer, M.H. 238 (1998) 179
- Walla, P.J., F. Jelezko, Ph. Tamarat, B. Lounis and M. Orrit, Perylene in biphenyl and anthracene crystals: an example of the influence of the host on single-molecule signals 233 (1998) 117
- Walla, P.J., see Nickel, B. 237 (1998) 371
- Wan, M., see Xiao, C. 237 (1998) 73
- Wang, C.H., see Qureshi, F.M. 231 (1998) 87
- Wang, L., A rigorous quantum molecular dynamics study of a collinear $A + BC \rightarrow AB + C$ reaction 237 (1998) 305
- Wang, M.-L., K.-L. Han, J.-P. Zhan, J.-H. Huang and G.-Z. He, Rotational alignment from the reactions $Sr(^3P_J) + CCl_4$ and $CHCl_3$ 236 (1998) 387
- Wang, M.-L., K.-L. Han, S.-L. Cong, G.-Z. He and N.-Q. Lou, Rotational alignment from the $Sr(^3P_J) + CH_2ClI$ chemiluminescent reaction 238 (1998) 481
- Wang, P.N., see Chen, J.H. 238 (1998) 165
- Wang, W. and A.J.C. Varandas, On the $O_2(v') + O_2(v'')$ atmospheric reaction. II. The role of rotational excitation 236 (1998) 181
- Wang, Z.G., see Chen, J.H. 238 (1998) 165
- Wannberg, B., see Baltzer, P. 237 (1998) 451
- Warda, S.A., see Hu, Z. 232 (1998) 63
- Warns, C., see Barvík, I. 240 (1999) 173
- Washida, N., see Zils, R. 231 (1998) 303
- Wasylyshyn, D.A. and G.P. Johari, Dielectric effects of step-increased pressure on the mass- and diffusion-controlled linear chain and network macromolecules growth 237 (1998) 345
- Watanabe, H. and T. Asada, Hybrid procedure of the ab initio molecular orbital (MO) method and the Monte Carlo samplings; application to cluster $B^+(H_2O)$ 237 (1998) 81

- Waterstradt, E., see Chapman, D.M. 239 (1998) 417
- Weber, J.M., K. Hansen, M.-W. Ruf and H. Hotop, Penning ionization of C₆₀ and C₇₀ 239 (1998) 271
- Weddle, G.H., see Ayotte, P. 239 (1998) 485
- Weinheimer, C.J. and J.M. Lisy, Vibrational and unimolecular dissociation of mixed solvent cluster ions: Na⁺((CH₃)₂CO)_n(CH₃OH)_m 239 (1998) 357
- Weinkauff, R., see Schiedt, J. 239 (1998) 511
- Weitzel, K.-M., Ab initio study of the equilibrium conformation of the ArCO⁺ ion 237 (1998) 43
- Welland, A.D., F.W. Schneider and A.B.J. Parusel, Dual fluorescence of the isoquinolinium cation in methanol: time-resolved emission spectra and semiempirical calculations 240 (1999) 403
- Wen, T.C., see Tsai, C.Y. 240 (1999) 191
- Werhahn, O., see Huisken, F. 239 (1998) 11
- Werner, H.-J., see Hartke, B. 239 (1998) 561
- Wichmann, D. and K. Jug, Decomposition of perchlorodisiloxane 236 (1998) 87
- Wiersma, D.A., see de Boeij, W.P. 233 (1998) 287
- Wilhelm, R., see Lindner, J. 238 (1998) 329
- Wine, P.H., see Piety, C.A. 231 (1998) 155
- Wolf, U., see Borsenberger, P.M. 234 (1998) 277
- Wolfseder, B., L. Seidner, W. Domcke, G. Stock, M. Seel, S. Engleitner and W. Zinth, Vibrational coherence in ultrafast electron-transfer dynamics of oxazine 1 in N,N-dimethylaniline: simulation of a femtosecond pump-probe experiment 233 (1998) 323
- Xiao, C., K. Feng, Y. Mo, Q. Meng, M. Zhang, M. Wan and J. Zhao, The electronic structure and Raman spectroscopy of the first purely organic ferromagnet: β para-nitrophenyl nitronyl nitroxide 237 (1998) 73
- Xu, H., see Deng, H. 231 (1998) 95
- Xue, B., see DeRose, P. 239 (1998) 235
- Yagi, T., H. Takase, K. Morihashi and O. Kikuchi, Monte Carlo and molecular orbital study of solvent effect on the electronic structure and hyperfine coupling constants of the (CH₃)₂NO radical: the effect of electron transfer between the solute and solvent molecules 232 (1998) 1
- Yamanouchi, K., see Hishikawa, A. 231 (1998) 315
- Yan, Y.J., Z.W. Shen and Y. Zhao, Optimal pump-dump control: phase-locked versus phase-unlocked schemes 233 (1998) 191
- Yang, D.-Y., see Berezhkovskii, A.M. 235 (1998) 201
- Yang, L., see Magnuson, M. 237 (1998) 295
- Yang, M.M., see Kummer, A.D. 237 (1998) 183
- Yang, X., I. Gerasimov and P.J. Dagdigan, Electronic spectroscopy and excited state dynamics of the Al-N₂ complex 239 (1998) 207
- Yasuda, T. and S.-i. Ikawa, On the dielectric continuum solvent model for theoretical estimates of the conformational equilibrium of molecules with an intramolecular hydrogen bond 238 (1998) 173
- Yeager, D.L., see McKellar, A.J. 238 (1998) 1
- Yencha, A.J., A.J. Cormack, R.J. Donovan, A. Hopkirk and G.C. King, Threshold photoelectron spectroscopy of HCl and DCl 238 (1998) 109
- Yencha, A.J., A.J. Cormack, R.J. Donovan, K.P. Lawley, A. Hopkirk and G.C. King, Threshold photoelectron spectroscopy of HBr and DBr 238 (1998) 133
- Yi, X., see Guan, D. 233 (1998) 35

- Yonekura, N., see Katayanagi, H. 231 (1998) 345
Yoshihara, K., see Shirota, H. 236 (1998) 355
Youvan, D.C., see Kummer, A.D. 237 (1998) 183
Yu, Z., see Huang, W. 237 (1998) 223
- Zacharias, H., see Menzel, C. 239 (1998) 287
Zadayan, R., N. Schwentner and V.A. Apkarian, Wavepacket diagnosis with chirped probe pulses 233 (1998) 353
Žagar, V., see Seliger, J. 234 (1998) 223
Zaika, V., see Kadashchuk, A. 234 (1998) 285
Zerbe, C., see Shao, J. 235 (1998) 81
Zerbetto, F., see Bini, R. 232 (1998) 75
Zerbetto, F., see Brouwer, A.M. 238 (1998) 421
Zhan, J.-P., see Wang, M.-L. 236 (1998) 387
Zhang, M., see Xiao, C. 237 (1998) 73
Zhang, Y., see Huang, W. 237 (1998) 223
Zhao, H., see Gingell, J.M. 237 (1998) 443
Zhao, J., see Xiao, C. 237 (1998) 73
Zhao, Y., see Yan, Y.J. 233 (1998) 191
Zhong, Q., see Poth, L. 239 (1998) 309
Zhou, T., see Cundari, T.R. 240 (1999) 205
Zhu, L., see Fiss, J.A. 233 (1998) 335
Zils, R., S. Inomata, Y. Okunuki and N. Washida, Direct observation of the equilibrium between cyclohexenyl radicals, O₂, and cyclohexenylperoxy radicals 231 (1998) 303
Zimmermann, H., see Detken, A. 238 (1998) 301
Zinth, W., see Wolfseder, B. 233 (1998) 323
Zitserman, V.Yu., see Berezhkovskii, A.M. 235 (1998) 201
Zuhrt, C., R. Neumann and L. Zülicke, Investigation of vibrational states of the ArHCl⁺ cation in the electronic ground state 240 (1999) 117
Zülicke, L., see Zuhrt, C. 240 (1999) 117
Zuñiga, J., see Bastida, A. 240 (1999) 229
Zwier, J.M., see Brouwer, A.M. 238 (1998) 421
Zwier, T.S., see Hagemeister, F.C. 239 (1998) 83

Subject index to volumes 231–240

Methods and constructs

Theoretical

Computational methods for electronic structure

- Differential ring proton NMR shieldings and cyclic stabilization energies, D.B. Chesnut 231 (1998) 1
- Kinetic and mechanistic study of the reaction of atomic chlorine with methyl bromide over an extended temperature range, C.A. Piety, R. Soller, J.M. Nicovich, M.L. McKee and P.H. Wine 231 (1998) 155
- Spin-orbit branching in the predissociation of the $C^1\Pi$ state of HCl and DCl: a manifestation of quantum interference, M.H. Alexander, X. Li, R. Liyanage and R.J. Gordon 231 (1998) 331
- Monte Carlo and molecular orbital study of solvent effect on the electronic structure and hyperfine coupling constants of the $(CH_3)_2NO$ radical: the effect of electron transfer between the solute and solvent molecules, T. Yagi, H. Takase, K. Morihashi and O. Kikuchi 232 (1998) 1
- Theoretical study of X-ray circular dichroism of amino acids, O. Plashkevych, V. Caravetta, O. Vahtras and H. Ågren 232 (1998) 49
- On the electronic structure of Cu(III) and Ni(III) in $La_2Li_{1/2}Cu_{1/2}O_4$, $Nd_2Li_{1/2}Ni_{1/2}O_4$, and Cs_2KCuF_6 , Z. Hu, G. Kaindl, S.A. Warda, D. Reinen, F.M.F. de Groot and B.G. Müller 232 (1998) 63
- Bridged-assisted electron transfer. Random matrix theory approach, E. Gudowska-Nowak, G. Papp and J. Brickmann 232 (1998) 247
- Ab initio* study of excited-state intramolecular proton dislocation in salicylic acid, A.L. Sobolewski and W. Domcke 232 (1998) 257
- Accurate universal basis set for H through Xe for Hartree–Fock calculations, F.E. Jorge and R.F. Martins 233 (1998) 1
- Classical and quantum dynamics on the collinear potential energy surface for the reaction of Li with H_2 , N.J. Clarke, M. Sironi, M. Raimondi, S. Kumar, F.A. Gianturco, E. Buonomo and D.L. Cooper 233 (1998) 9
- Intramolecular proton transfer in the ground and the two lowest-lying singlet excited states of 1-amino-3-propenal and related species, M. Forés, M. Duran and M. Solà 234 (1998) 1
- Time-resolved resonance Raman and molecular orbital studies of charge separation and intramolecular reorganisation, G.D. Scholes, I.R. Gould, A.W. Parker and D. Phillips 234 (1998) 21

- Ab initio calculations and supersonic jet studies on the geometry of 4-dimethylamino-benzonitrile (DMABN) and related compounds in the ground and excited state, U. Lommatzsch and B. Brutschy 234 (1998) 35
- Electrical properties of a charged surface in a general electrolyte solution, Y.-C. Kuo and J.-P. Hsu 236 (1998) 1
- CARS studies of bending states of CO₂: evidence of collisional rotational transitions with odd ΔJ , A.P. Kouzov, D.N. Kozlov and B. Hemmerling 236 (1998) 15
- Franck–Condon effects in low-energy states of C₁₀H₈⁺ radical. Ab initio MCSCF study of absorption and resonance Raman spectra, T. Andruniow and M. Pawlikowski 236 (1998) 25
- Vibronic coupling effects in the low-energy 1²B_{1g} and 2²B_{1g} states of the C₁₀H₈⁺ radical, T. Andruniow and M. Pawlikowski 236 (1998) 35
- Ultraviolet absorption spectrum and cross-sections of vinyl (C₂H₃) radical in the 225–238 nm region, A. Fahr, P. Hassanzadeh and D.B. Atkinson 236 (1998) 43
- Decomposition of perchlorodisiloxane, D. Wichmann and K. Jug 236 (1998) 87
- A comparative study of the electronic structure of α -MnS (alabandite) calculated at the Hartree-Fock and Density Functional levels of theory, R. Tappero and A. Lichanot 236 (1998) 97
- The mechanism of the CH₃O + CO reaction and the stability of the CH₃OCO radical, J.S. Francisco 237 (1998) 1
- Classical energy calculations with electron correlation of condensed excited states — Rydberg Matter, L. Holmlid 237 (1998) 11
- Ab-initio CI calculations of the Cls and ClIs and 2p core excitation spectra of the freon molecules: CCl₄, CFCI₃, CF₂Cl₂ and CF₃Cl, G. Fronzoni and P. Decleva 237 (1998) 21
- Complete basis set ab initio study of monocomplexation of aluminum with H₂O, NH₃, and HF, B.S. Jursic 237 (1998) 51
- Model calculations of local exciton levels in the C₆₀ fullerene crystals doped with endohedral fullerenes M@C₆₀, A. Eilmes and P. Petelenz 237 (1998) 67
- The electronic structure and Raman spectroscopy of the first purely organic ferromagnet: β para-nitrophenyl nitronyl nitroxide, C. Xiao, K. Feng, Y. Mo, Q. Meng, M. Zhang, M. Wan and J. Zhao 237 (1998) 73
- Hybrid procedure of the ab initio molecular orbital (MO) method and the Monte Carlo samplings; application to cluster B⁺(H₂O), H. Watanabe and T. Asada 237 (1998) 81
- Correlation corrected energy bands of nucleotide base stacks, F. Bogár and J. Ladik 237 (1998) 273
- Complete basis set limit ionization potentials of O₃ and NO₂ using the multiconfigurational spin tensor electron propagator method (MCSTEP), A.J. McKellar, D. Heryadi, D.L. Yeager and J.A. Nichols 238 (1998) 1
- Analysis of the reaction paths to dissociation of dichloro-ethylenes into Cl₂ and C₂H₂, S.M. Resende and W.B. De Almeida 238 (1998) 11
- An ab initio time-dependent Hartree–Fock study of solvent effects on the polarizability and second hyperpolarizability of polyacetylene chains within the polarizable continuum model, B. Champagne, B. Mennucci, M. Cossi, R. Cammi and J. Tomasi 238 (1998) 153
- The first-order electric field-induced spectra: theory and experimental study of NO₂, J.H. Chen, P.N. Wang, F.M. Li, Y.Q. Chen and Z.G. Wang 238 (1998) 165
- On the dielectric continuum solvent model for theoretical estimates of the conformational equilibrium of molecules with an intramolecular hydrogen bond, T. Yasuda and S.-i. Ikawa 238 (1998) 173
- The electronic states of pyrrole studied by optical (VUV) absorption, near-threshold electron energy-loss (EEL) spectroscopy and ab initio multi-reference configuration interaction calculations, M.H. Palmer, I.C. Walker and M.F. Guest 238 (1998) 179

- Inner-shell excitation of PF_3 , PCl_3 , PCl_2CF_3 , OPF_3 and SPF_3 . Part I. Spectroscopy, J.J. Neville, A. Jürgensen, R.G. Cavell, N. Kosugi and A.P. Hitchcock 238 (1998) 201
- Mass spectrometric and theoretical study of the mixed complex $\text{NaCeCl}_4(\text{g})$, J. Kapala, S. Roszak, I. Lisek and M. Miller 238 (1998) 221
- Solvent effects within the CS INDO method. Geometrical distortion and solvatochromism of merocyanine dyes, I. Baraldi, F. Momicchioli, G. Ponterini and D. Vanossi 238 (1998) 353
- Cold photoconductivity in a system of interacting charge-transfer excitons at a donor–acceptor interface, S.A. Kiselev, E. Hartung, Z.G. Soos, S.R. Forrest and V.M. Agranovich 238 (1998) 365
- Non-orthogonal orbitals for localized electrons. I. The Spin-Coupled wavefunction, A. Fritsch 238 (1998) 373
- Investigations of OH–N- and NH–O-type hydrogen-bonded clusters by UV laser spectroscopy, C. Jacoby, P. Hering, M. Schmitt, W. Roth and K. Kleinermanns 239 (1998) 23
- Structure and dynamics of the phenol–water–argon cation radical, D.M. Chapman, F.J. Hompf, K. Müller-Dethlefs, E. Waterstradt, P. Hobza and V. Špirko 239 (1998) 417
- Many-body exchange effects in clusters of rare gases with a chromophore: He_2CO_2 , J. Jakowski, G. Chałasiński, M.M. Szcześniak and S.M. Cybulski 239 (1998) 573
- Ab initio theoretical optical rotations of small molecules, P.L. Polavarapu and D.K. Chakraborty 240 (1999) 1
- Ab initio study of the amino group twisting and wagging reaction paths in the intramolecular charge transfer of 4-(N,N-dimethylamino)benzonitrile, W. Sudholt, A.L. Sobolewski and W. Domcke 240 (1999) 9
- Diatomics-in-molecules applied to solid hydrogen doped with $\text{O}(^1D_g)$, P.J. Kuntz 240 (1999) 19
- Electron paramagnetic resonance of Er^{3+} doped in YVO_4 : hyperfine parameters, S.K. Misra, S. Isber, J.A. Capobianco and E. Cavalli 240 (1999) 313
- CI and valence bond approach*
- Quantum chemical modeling of structure and absorption spectra of the chromophore in green fluorescent proteins, A.A. Voityuk, M.-E. Michel-Beyerle and N. Rösch 231 (1998) 13
- Theoretical study of the Cl 1s and 2p near edge photoabsorption spectra of HCl by accurate ab-initio configuration interaction and density functional approaches, G. Fronzoni, M. Stener, P. Decleva and G. De Alti 232 (1998) 9
- Bonding in molecular dications from the classical valence bond viewpoint. A case study of CO^{2+} , R. Polák 232 (1998) 25
- A Valence-Bond/Hartree–Fock method to determine the Hubbard transfer integrals in organic conductors, F. Castet, L. Ducasse and A. Fritsch 232 (1998) 37
- Ab-initio study of a radiative association mechanism application to the $\text{CH}_3^+ + \text{H}_2$ reaction, D. Talbi and M.C. Bacchus-Montabonel 232 (1998) 267
- Hartree–Fock limit properties of the water dimer in absence of BSSE, A. Famulari, M. Raimondi, M. Sironi and E. Gianinetti 232 (1998) 275
- Ab initio MO–VB study of water dimer, A. Famulari, M. Raimondi, M. Sironi and E. Gianinetti 232 (1998) 289
- Ab initio study of the $X^2\Sigma^+$ and $A^2\Pi$ states of the SiO^+ cation including the effect of core correlation, Z.-L. Cai and J.P. François 234 (1998) 59
- Theoretical study of the ethylene radical cation: geometry and hyperfine structure, N. Salhi-Benachenhou, B. Engels, M.-B. Huang and S. Lunell 236 (1998) 53
- Ab-initio CI calculations of the Cl 1s and Cl 1s and 2p core excitation spectra of the freon molecules: CCl_4 , CFCl_3 , CF_2Cl_2 and CF_3Cl , G. Fronzoni and P. Decleva 237 (1998) 21

- Ab initio study of the equilibrium conformation of the ArCO^+ ion, K.-M. Weitzel 237 (1998) 43
- Complete basis set ab initio study of monocomplexation of aluminum with H_2O , NH_3 , and HF , B.S. Jursic 237 (1998) 51
- Theoretical study of the crystal field excitations in CoO , C. de Graaf, W.A. de Jong, R. Broer and W.C. Nieuwpoort 237 (1998) 59
- Charge transfer recombination of Si^{2+} ions from atomic hydrogen, M.C. Bacchus-Montabonel 237 (1998) 245
- Matrix photochemistry of nitrosyl chloride. Interconversion of ClNO and ClON species by irradiation and tunneling effect, A. Hallou, L. Schriver-Mazzuoli, A. Schriver and P. Chaquin 237 (1998) 251
- The vibrational and temperature dependence of the indirect nuclear spin–spin coupling constants of the oxonium (H_3O^+) and hydroxyl (OH^-) ions, S.P.A. Sauer, C.K. Møller, H. Koch, I. Paidarová and V. Špirko 238 (1998) 385
- Charge transfer between Si^{3+} and helium at thermal and low energies, P. Honvault, M.C. Bacchus-Montabonel, M. Gargaud and R. McCarroll 238 (1998) 401
- Analysis of a nonlinear optical response of CN^- ions adsorbed on metal electrode: tentative interpretation by means of ab initio molecular calculations, M. Tadjeddine and J.P. Flament 240 (1999) 39
- A gas phase ab initio excited state geometry optimization study of thymine, cytosine and uracil, M.K. Shukla and P.C. Mishra 240 (1999) 319
- Dual fluorescence of the isoquinolinium cation in methanol: time-resolved emission spectra and semiempirical calculations, A.D. Welland, F.W. Schneider and A.B.J. Parusel 240 (1999) 403
- perturbative and many body approaches*
- Theoretical study of the $\text{Cl } 1s$ and $2p$ near edge photoabsorption spectra of HCl by accurate ab-initio configuration interaction and density functional approaches, G. Fronzoni, M. Stener, P. Decleva and G. De Alti 232 (1998) 9
- An ab initio study of NMR isotropic shielding bond length derivatives in phosphorus compounds, A. Dransfeld and D.B. Chesnut 234 (1998) 69
- Theoretical study of the ethylene radical cation: geometry and hyperfine structure, N. Salhi-Benachenhrou, B. Engels, M.-B. Huang and S. Lunell 236 (1998) 53
- Electrical interaction between two spherical particles covered by an ion-penetrable charged membrane, J.-P. Hsu and B.-T. Liu 236 (1998) 63
- Study of positronium hydride with a simple wavefunction: Application to the Stark effect of PsH , C. Le Sech and B. Silvi 236 (1998) 77
- Decomposition of perchlorodisiloxane, D. Wichmann and K. Jug 236 (1998) 87
- Theoretical study of the crystal field excitations in CoO , C. de Graaf, W.A. de Jong, R. Broer and W.C. Nieuwpoort 237 (1998) 59
- Vertical double ionization of the sulphur dioxide molecule, I.W. Griffiths, D.E. Parry and F.M. Harris 238 (1998) 21
- The vibrational and temperature dependence of the indirect nuclear spin–spin coupling constants of the oxonium (H_3O^+) and hydroxyl (OH^-) ions, S.P.A. Sauer, C.K. Møller, H. Koch, I. Paidarová and V. Špirko 238 (1998) 385
- Improved intermolecular water potential from global geometry optimization of small water clusters using local MP2, B. Hartke, M. Schütz and H.-J. Werner 239 (1998) 561
- density functional theory*
- Theoretical study of the $\text{Cl } 1s$ and $2p$ near edge photoabsorption spectra of HCl by accurate ab-initio configuration interaction and density functional approaches, G. Fronzoni, M. Stener, P. Decleva and G. De Alti 232 (1998) 9

- A density functional study of weakly bound hydrogen bonded complexes, A.K. Chandra and M.T. Nguyen 232 (1998) 299
- Infrared spectra of polycyclic aromatic hydrocarbons: oxygen substitution, C.W. Bauschlicher, Jr. 233 (1998) 29
- Ab initio study of the $X^2\Sigma^+$ and $A^2\Pi$ states of the SiO^+ cation including the effect of core correlation, Z.-L. Cai and J.P. François 234 (1998) 59
- Infrared spectra of polycyclic aromatic hydrocarbons: methyl substitution and loss of H, C.W. Bauschlicher, Jr. and S.R. Langhoff 234 (1998) 79
- Infrared spectra of polycyclic aromatic hydrocarbons: nitrogen substitution, C.W. Bauschlicher, Jr. 234 (1998) 87
- Valence photoionization of C_6H_6 by the B-spline one-centre expansion density functional method, M. Venuti, M. Stener and P. Decleva 234 (1998) 95
- A comparative study of the electronic structure of $\alpha\text{-MnS}$ (alabandite) calculated at the Hartree-Fock and Density Functional levels of theory, R. Tappero and A. Lichanot 236 (1998) 97
- Model calculations of local exciton levels in the C_{60} fullerene crystals doped with endohedral fullerenes M@C_{60} , A. Eilmes and P. Petelenz 237 (1998) 67
- Infrared spectra and theoretical calculations of HCl complexed with NO , L. Krim and M.E. Alikhani 237 (1998) 265
- Vibrational analysis of 2-nitrophenol. A joint FT-IR, FT-Raman and scaled quantum mechanical study, A. Kovács, V. Izvekov, G. Keresztury and G. Pongor 238 (1998) 231
- Chemical bonding and magnetic properties of the high-spin molecule $[\text{Mn}_{12}\text{O}_{12}(\text{HCOO})_{16}(\text{H}_2\text{O})_4]$, Y. Duan 238 (1998) 407
- Analysis of a nonlinear optical response of CN^- ions adsorbed on metal electrode: tentative interpretation by means of ab initio molecular calculations, M. Tadjeddine and J.P. Flament 240 (1999) 39
- Infrared absorption and Raman scattering of (Z)-3-hydroxypropenal. A density functional theoretical study, J. Spanget-Larsen 240 (1999) 51
- L-Alanyl-L-alanine in the zwitterionic state: structures determined in the presence of explicit water molecules and with continuum models using density functional theory, M. Knapp-Mohammady, K.J. Jalkanen, F. Nardi, R.C. Wade and S. Suhai 240 (1999) 63

Semiempirical methods

- Quantum chemical modeling of structure and absorption spectra of the chromophore in green fluorescent proteins, A.A. Voityuk, M.-E. Michel-Beyerle and N. Rösch 231 (1998) 13
- Generalization of the Arrhenius relation and ionization reaction rates for carbon atoms and ions in plasmas, Y. Chang and C.A. Ordonez 231 (1998) 27
- A Valence-Bond/Hartree-Fock method to determine the Hubbard transfer integrals in organic conductors, F. Castet, L. Ducasse and A. Fritsch 232 (1998) 37
- The vibrational spectroscopy of $\text{C}_{60}\text{H}_{36}$: An experimental and theoretical study, R. Bini, J. Ebenhoch, M. Fanti, P.W. Fowler, S. Leach, G. Orlandi, Ch. Rüchardt, J.P.B. Sandall and F. Zerbetto 232 (1998) 75
- Effect of the angular dependence of the barrier height on the features of the $\text{F} + \text{H}_2$ reaction, V.M. Azriel, L.Yu. Rusin, M.B. Sevryuk and J.P. Toennies 232 (1998) 307
- Towards quantitative diatomics-in-molecules model for the water molecule, B.L. Grigorenko, A.V. Nemukhin and V.A. Apkarian 232 (1998) 321
- Modelling aluminium clusters with an empirical many-body potential, L.D. Lloyd and R.L. Johnston 236 (1998) 107

- Modelling the substitution effects of several rhodium(III) transition metal complexes using the angular overlap model, B. Gilliams, D. Vandenbroucke and C. Görrler-Walrand 237 (1998) 91
- Structure of the Van der Waals rare gas–C₆₀ exohedral complexes [(C₆₀)(RG)_n; n = 1, 2], S. Iglesias-Groth, J. Breton and C. Girardet 237 (1998) 285
- Neutral and negatively-charged formamide, N-methylformamide and dimethylformamide clusters, C. Desfrancois, V. Périquet, S. Carles, J.P. Schermann and L. Adamowicz 239 (1998) 475
- Modeling structure and dynamics of solvated molecular ions: Photodissociation and recombination in I₂[−](CO₂)_n, J. Faeder, N. Delaney, P.E. Maslen and R. Parson 239 (1998) 525
- Calculation of structures and vibrational spectra of acetonitrile clusters, J.G. Siebers, U. Buck and T.A. Beu 239 (1998) 549
- Diatomics-in-molecules applied to solid hydrogen doped with O(¹D_g), P.J. Kuntz 240 (1999) 19
- DIM models for RgX₂[−] systems: suppressed influence of spin-orbit coupling and induced multipole effects for the Ar–I₂[−] interaction, F.Y. Naumkin 240 (1999) 79
- Effect of solvent fluctuations on proton transfer dynamics: a hybrid AM1/MM molecular dynamics simulation on the [H₃N–H–NH₃]⁺ system, G.-S. Li, M.T.C. Martins Costa, C. Millot and M.F. Ruiz-López 240 (1999) 93
- Molecular modelling study for chiral separation of equol enantiomers by β-cyclodextrin, E. Alvira, J.I. García and J.A. Mayoral 240 (1999) 101
- Dual fluorescence of the isoquinolinium cation in methanol: time-resolved emission spectra and semiempirical calculations, A.D. Welland, F.W. Schneider and A.B.J. Parusel 240 (1999) 403
- Algebraic approaches*
- Bridged-assisted electron transfer. Random matrix theory approach, E. Gudowska-Nowak, G. Papp and J. Brickmann 232 (1998) 247
- Water anomalies and the double-well Takahashi model, C.H. Cho, S. Singh and G.W. Robinson 232 (1998) 329
- Yamanouchi-chain \mathcal{S}_n -invariant hierarchies for SR carrier space of $\{T^k(v)\}(SU2 \times \mathcal{S}_n)$ dual tensors in NMR: some maximal \mathcal{S}_n -inner products, via \mathcal{S}_n -restricted-space Schur Fn. product mappings, F.P. Temme 238 (1998) 245
- Experimental and theoretical studies of the low-lying electronic states of the simplest benzylic amide [2]catenane, A.M. Brouwer, W.J. Buma, R. Caudano, M. Fanti, C.-A. Fustin, D.A. Leigh, A. Murphy, P. Rudolf, F. Zerbetto and J.M. Zwieter 238 (1998) 421
- Relativistic electronic structure theory*
- Theoretical study of the crystal field excitations in CoO, C. de Graaf, W.A. de Jong, R. Broer and W.C. Nieuwpoort 237 (1998) 59
- On the accuracy of averaged relativistic shape-consistent pseudopotentials, L. Maron and C. Teichteil 237 (1998) 105
- DIM models for RgX₂[−] systems: suppressed influence of spin-orbit coupling and induced multipole effects for the Ar–I₂[−] interaction, F.Y. Naumkin 240 (1999) 79
- Wavefunctions for highly excited and unbound states*
- Theoretical study of X-ray circular dichroism of amino acids, O. Plashkevych, V. Caravetta, O. Vahtras and H. Ågren 232 (1998) 49
- A theoretical study of the electronic structure and spectroscopic properties of the low-lying electronic states of the molecule AlSi, F.R. Ornellas and S. Iwata 232 (1998) 95
- A semiclassical study of dissociation dynamics in He + H₂ collisions, K. Sakimoto 236 (1998) 123

- Vibrationally state-selective laser pulse control of electronic branching in OH ($X^2\Pi/A^2\Sigma^+$) photoassociation, M.V. Korolkov and B. Schmidt 237 (1998) 123
- Ab initio study of the electronic spectrum of $C_2H_2^+$. I. Vertical spectrum and angular potential curves, M. Perić, B. Engels and M. Hanrath 238 (1998) 33
- Ab initio study of the electronic spectrum of $C_2H_2^+$. II. Stretching potential energy surfaces for low-lying doublet electronic states, M. Perić and B. Engels 238 (1998) 47
- On librational broadening of vibrational transitions in liquids: a simple model, D.J. Ulness, J.C. Kirkwood and A.C. Albrecht 240 (1999) 109
- Investigation of vibrational states of the $ArHCl^+$ cation in the electronic ground state, C. Zuhrt, R. Neumann and L. Zülicke 240 (1999) 117
- Control of transition state spectra: a variational algorithm, R.T. Skodje, R. Sadeghi and J.L. Krause 240 (1999) 129
- Spin states and magnetic interactions*
- Differential ring proton NMR shieldings and cyclic stabilization energies, D.B. Chesnut 231 (1998) 1
- An ab initio study of NMR isotropic shielding bond length derivatives in phosphorus compounds, A. Dransfeld and D.B. Chesnut 234 (1998) 69
- Solvent effects on NMR spectrum of acetylene calculated by ab initio methods, M. Pecul and J. Sadlej 234 (1998) 111
- Suppression of quantum coherence: Noise effect, J. Shao, C. Zerbe and P. Hänggi 235 (1998) 81
- A comparative study of the electronic structure of α -MnS (alabandite) calculated at the Hartree-Fock and Density Functional levels of theory, R. Tappero and A. Lichanot 236 (1998) 97
- Electronic structure of planar superconducting systems. From finite to extended model, S. Larsson 236 (1998) 133
- The electronic structure and Raman spectroscopy of the first purely organic ferromagnet: β para-nitrophenyl nitronyl nitroxide, C. Xiao, K. Feng, Y. Mo, Q. Meng, M. Zhang, M. Wan and J. Zhao 237 (1998) 73
- Yamanouchi-chain \mathcal{S}_n -invariant hierarchies for SR carrier space of $\{T^k(v)\}(SU2 \times \mathcal{S}_n)$ dual tensors in NMR: some maximal \mathcal{S}_n -inner products, via \mathcal{S}_n -restricted-space Schur Fn. product mappings, F.P. Temme 238 (1998) 245
- Chemical bonding and magnetic properties of the high-spin molecule $[Mn_{12}O_{12}(HCOO)_{16}(H_2O)_4]$, Y. Duan 238 (1998) 407
- Radical-substituted allenes as high-spin species and subunits of organic ferromagnets, R. Beust, N. Tyutyulkov, M. Rabinovitz and F. Dietz 240 (1999) 141
- Localisation vs. delocalisation in the dimeric mixed-valence clusters in the generalised vibronic model. Magnetic manifestations, J.J. Borrás-Almenar, E. Coronado, S.M. Ostrovsky, A.V. Palii and B.S. Tsukerblat 240 (1999) 149
- Molecular response to external fields (incl. optical susceptibilities, dichroism, hyperpolarizabilities)*
- Ultrafast laser control of vibrational dynamics for a two-dimensional model of $HONO_2$ in the ground electronic state: separation of conformers, control of the bond length, selective preparation of the discrete and the continuum states, M. Oppel and G.K. Paramonov 232 (1998) 111
- Ab initio variational calculation of dynamic polarizabilities and hyperpolarizabilities. I. Polarizability and quadratic hyperpolarizability of water, carbon monoxide and hydrogen fluoride, A. Lembarki, C. Barbier, Ph. Lemaire and E.N. Svendsen 232 (1998) 343
- Optimal pump-dump control: phase-locked versus phase-unlocked schemes, Y.J. Yan, Z.W. Shen and Y. Zhao 233 (1998) 191

- Controlling condensed-phase vibrational excitation with tailored infrared pulses, V.D. Kleiman, S.M. Arrivo, J.S. Melinger and E.J. Heilweil 233 (1998) 207
- Wavepacket diagnosis with chirped probe pulses, R. Zadoyan, N. Schwentner and V.A. Apkarian 233 (1998) 353
- Suppression of quantum coherence: Noise effect, J. Shao, C. Zerbe and P. Hänggi 235 (1998) 81
- Field-induced localization and nonlinear response of a one-band conductor to a periodic electric field, A.A. Ovchinnikov and K.A. Pronin 235 (1998) 93
- Role of the local electric field in electro-absorption spectra of molecular crystals, R.W. Munn 236 (1998) 151
- Linear response calculations of electronic *g*-factors and spin-rotational coupling constants for diatomic molecules with a triplet ground state, M. Engström, B. Minaev, O. Vahtras and H. Ågren 237 (1998) 149
- An ab initio time-dependent Hartree–Fock study of solvent effects on the polarizability and second hyperpolarizability of polyacetylene chains within the polarizable continuum model, B. Champagne, B. Mennucci, M. Cossi, R. Cammi and J. Tomasi 238 (1998) 153
- Wavelength dependence of the nonlinear absorption properties of laser dyes in solid and liquid solutions, J. Barroso, A. Costela, I. García-Moreno and R. Sastre 238 (1998) 257
- The vibrational and temperature dependence of the indirect nuclear spin–spin coupling constants of the oxonium (H_3O^+) and hydroxyl (OH^-) ions, S.P.A. Sauer, C.K. Møller, H. Koch, I. Paidarová and V. Špirko 238 (1998) 385
- The study on the magnetic field effect and the microwave effect on the photoconductivity observed in the photolysis of *N,N,N',N'*-tetramethyl-*p*-phenylenediamine: theoretical calculation trial by the stochastic Liouville equation, Y. Kitahama and H. Murai 238 (1998) 429
- Analysis of a nonlinear optical response of CN^- ions adsorbed on metal electrode: tentative interpretation by means of ab initio molecular calculations, M. Tadjeddine and J.P. Flament 240 (1999) 39
- Infrared absorption and Raman scattering of (Z)-3-hydroxypropenal. A density functional theoretical study, J. Spanget-Larsen 240 (1999) 51
- Laser driven hydrogen tunneling in a dissipative environment, H. Naundorf, K. Sundermann and O. Kühn 240 (1999) 163
- Simulation of excitonic optical line shapes of cyclic molecular aggregates with 9 and 18 units: influence of quasi-static and dynamic disorder, I. Barvák, C. Warns, T. Neidlinger and P. Reineker 240 (1999) 173
- Nonlinear absorption and refraction in porphyrazine derivatives, C.Y. Tsai, S.P. Chen and T.C. Wen 240 (1999) 191
- Hole transport in arylamine doped polymers, S.A. Visser, W.T. Gruenbaum, E.H. Magin and P.M. Borsenberger 240 (1999) 197
- Modeling nonlinear optical properties of inorganic complexes. Counterion effects, T.R. Cundari, H.A. Kurtz and T. Zhou 240 (1999) 205
- Radiative (incl. relativistic) effects on molecules and molecular processes*
- Fluorescence lifetime of rovibrational states of h_4 -acetaldehyde and spectra of d_4 -acetaldehyde, S.-H. Jen, T.-J. Hsu and I.-C. Chen 232 (1998) 131
- Ab-initio study of a radiative association mechanism application to the $\text{CH}_3^+ + \text{H}_2$ reaction, D. Talbi and M.C. Bacchus-Montabonel 232 (1998) 267
- Optimal pump-dump control: phase-locked versus phase-unlocked schemes, Y.J. Yan, Z.W. Shen and Y. Zhao 233 (1998) 191
- Interplay of creation, propagation, and relaxation of an excitation in a dimer, J. Peřina, Jr. 236 (1998) 157

- Vibrationally state-selective laser pulse control of electronic branching in OH ($X^2\Pi/A^2\Sigma^+$) photoassociation, M.V. Korolkov and B. Schmidt 237 (1998) 123
- New investigation of the photodissociation of the HBr molecule: total cross-section, anisotropy parameter and dependence of the spin-orbit branching on the ground state vibrational level, B. Pouilly and M. Monnerville 238 (1998) 437
- Scattering of waves and particles*
- The correlation between the statistical properties of surface defect distribution and the specular intensity obtained from low energy He scattering technique, G. Petrella, L. Cassidei and F. Ciriaco 231 (1998) 31
- Charge transfer in gas-surface scattering: the three electronic state system, D. Guan, X. Yi, S. Ding, L. Gu and J.A. Olson 233 (1998) 35
- A semiclassical study of dissociation dynamics in He + H₂ collisions, K. Sakimoto 236 (1998) 123
- Theoretical study of the effect of reagent rotation and vibration on the reactions of Cl + H₂ and Cl + HD, J.-B. Song and E.A. Gislason 237 (1998) 159
- The electronic structure of poly(pyridine-2,5-diyl) investigated by soft X-ray absorption and emission spectroscopies, M. Magnuson, L. Yang, J.-H. Guo, C. S  the, A. Agui, J. Nordgren, Y. Luo, H.   gren, N. Johansson, W.R. Salaneck, L.E. Horsburgh and A.P. Monkman 237 (1998) 295
- Quantum study of oriented NO scattering from Ag(111): orientational steering and effects of surface corrugation, D. Lemoine and T. Duhoo 238 (1998) 59
- Semiclassical reactive scattering: the Hermite correction method in hyperspherical coordinates, S. Adhikari and G.D. Billing 238 (1998) 69
- Control of transition state spectra: a variational algorithm, R.T. Skodje, R. Sadeghi and J.L. Krause 240 (1999) 129
- Frenkel exciton scattering at microcrystallite surfaces caused by electric dipoles and monopoles, M. Takeshima and A.H. Matsui 240 (1999) 413
- Collisional and reactive molecular dynamics with non-frictional forces*
- Classical and quantum dynamics on the collinear potential energy surface for the reaction of Li with H₂, N.J. Clarke, M. Sironi, M. Raimondi, S. Kumar, F.A. Gianturco, E. Buonomo and D.L. Cooper 233 (1998) 9
- Polarisation effects in electronically inelastic collisions: SiFC²Δ + H₂ → SiFB²Σ⁺ + H₂, N.A. Jackson, C.J. Randall and K.G. McKendrick 233 (1998) 45
- A semiclassical study of dissociation dynamics in He + H₂ collisions, K. Sakimoto 236 (1998) 123
- On the O₂(*v*') + O₂(*v*') atmospheric reaction. II. The role of rotational excitation, W. Wang and A.J.C. Varandas 236 (1998) 181
- The mechanism of energy transfer in H₂O–H₂O collisions – a molecular dynamics simulation, H. Svedung, L.E.B. B  rjesson, N. Markovi   and S. Nordholm 236 (1998) 189
- Theoretical study of the effect of reagent rotation and vibration on the reactions of Cl + H₂ and Cl + HD, J.-B. Song and E.A. Gislason 237 (1998) 159
- Charge transfer recombination of Si²⁺ ions from atomic hydrogen, M.C. Bacchus-Montabonel 237 (1998) 245
- A rigorous quantum molecular dynamics study of a collinear A + BC → AB + C reaction, L. Wang 237 (1998) 305
- Interaction anisotropy and quantum dynamics for vibrationally inelastic collisions of LiH(¹Σ) with He(¹S), E. Bodo, E. Buonomo, F.A. Gianturco, S. Kumar, A. Famulari, M. Raimondi and M. Sironi 237 (1998) 315

- Charge transfer between Si^{3+} and helium at thermal and low energies, P. Honvault, M.C. Bacchus-Montabonel, M. Gargaud and R. McCarroll 238 (1998) 401
- Capture dynamics in collisions between fullerene ions and rare gas atoms, E.E.B. Campbell, R. Ehlich, G. Heusler, O. Knospe and H. Sprang 239 (1998) 299
- Reactive molecular dynamics including dissipative processes*
- Theoretical study of the $\text{OH} + \text{NO}_2$ reaction: formation of nitric acid and the hydroperoxyl radical, D. Chakraborty, J. Park and M.C. Lin 231 (1998) 39
- Direct observation of the equilibrium between cyclohexenyl radicals, O_2 , and cyclohexenylperoxy radicals, R. Zils, S. Inomata, Y. Okunuki and N. Washida 231 (1998) 303
- Fluorescence lifetime of rovibrational states of h_4 -acetaldehyde and spectra of d_4 -acetaldehyde, S.-H. Jen, T.-J. Hsu and I.-C. Chen 232 (1998) 131
- Dependence of volume-produced H^- ions on the wall recombination probability of H atoms in a low pressure H_2 positive column, J. Loureiro and J. Amorim 232 (1998) 141
- Effect of the angular dependence of the barrier height on the features of the $\text{F} + \text{H}_2$ reaction, V.M. Azriel, L.Yu. Rusin, M.B. Sevryuk and J.P. Toennies 232 (1998) 307
- Laser photodissociation of ketene at 230 nm, M. Castillejo, S. Couris, E. Lane, M. Martin and J. Ruiz 232 (1998) 353
- Transport properties of a reacting gas mixture with strong vibrational and chemical nonequilibrium, E.V. Kustova and E.A. Nagnibeda 233 (1998) 57
- Model study of proton transfer in a H-bonded cluster with an $\text{A}-\text{H}\cdots\text{B}$ reaction complex. Introduction of an effective coordinate for the solvation shell, M.V. Vener 233 (1998) 77
- Vibrational coherence in ultrafast electron-transfer dynamics of oxazine 1 in N,N-dimethylaniline: simulation of a femtosecond pump-probe experiment, B. Wolfseder, L. Seidner, W. Domcke, G. Stock, M. Seel, S. Engleitner and W. Zinth 233 (1998) 323
- The steady-state Green's function theory in monomolecular reactions. II. Effects of solvent dynamics and non-equilibrium initial distributions in reactions on position-dependent transition regions, O.B. Jenkins and A.B. Doktorov 234 (1998) 121
- Suppression of quantum coherence: Noise effect, J. Shao, C. Zerbe and P. Hänggi 235 (1998) 81
- Binary collision theory for thermal and nonisothermal relaxation and reaction of polyatomic molecules, P. Talkner, E. Pollak and A.M. Berezhkovskii 235 (1998) 131
- On the role of the energy loss in turnover theories of activated rate processes, A.N. Drozdov and J.J. Brey 235 (1998) 147
- Curvilinear-path based theory of the energy transfer limited rate of a two-dimensional solute in a dissipative bath, S.K. Reese and S.C. Tucker 235 (1998) 171
- Saddle point avoidance due to inhomogeneous friction, G.J. Moro and F. Cardin 235 (1998) 189
- Phase space distribution function approach to the Kramers problem. III. Anharmonic potentials, J. Morelli and D.J. Tannor 235 (1998) 213
- Nonadiabatic reactions in condensed phase in the absence of thermal equilibrium, I. Rips 235 (1998) 243
- Non-adiabatic effects in condensed phase activated rate processes in the near-adiabatic limit, A.I. Shushin and M. Tachiya 235 (1998) 267
- Non-equilibrium interlevel transitions in condensed phase far away from the avoided crossing region, M.V. Basilevsky, A.V. Soudackov and A.I. Voronin 235 (1998) 281
- Femtosecond pump-probe studies of chlorine dioxide photochemistry in water and acetonitrile, M.J. Philpott, S.C. Hayes and P.J. Reid 236 (1998) 207
- A simple analytical estimate of the bound-free Franck-Condon factors for a transition to a repulsive exponential potential in a diatomic molecule, V. Brems 238 (1998) 85
- Effects of complex formation on reactions of oxygen with HCl and $\text{Ar}-\text{HCl}$, M.W. Lufaso and A.B. McCoy 239 (1998) 187

- Laser driven hydrogen tunneling in a dissipative environment, H. Naundorf, K. Sundermann and O. Kühn 240 (1999) 163
- Contributions to the spectroscopic–kinetic analysis of linear reaction systems. Systems with three linearly independent reactions using the concept of parallel projection, J. Polster 240 (1999) 331
- Intramolecular dynamics*
- ¹³C NMR relaxation in neutral and charged tetra-*n*-alkyl compounds, B. Bordes, F. Coletta, A. Ferrarini, F. Gottardi and P.L. Nordio 231 (1998) 51
- Solvation of chromone using combined Discrete/SCRF models, C. Alemán and S.E. Galembeck 232 (1998) 151
- Pathway approach to ultrafast photochemistry: potential surfaces, conical intersections and isomerizations of small polyenes, W. Fuß, S. Lochbrunner, A.M. Müller, T. Schikarski, W.E. Schmid and S.A. Trushin 232 (1998) 161
- Tunneling splittings in vibrational spectra of non-rigid molecules: III. Tunneling coordinate-dependent coupling between small amplitude motions, V.A. Benderskii, E.V. Vetoshkin and H.P. Trommsdorff 234 (1998) 153
- Tunneling splittings in vibrational spectra of non-rigid molecules. IV. Kinematic couplings, V.A. Benderskii and E.V. Vetoshkin 234 (1998) 173
- REMPI spectroscopy of internal state populations in HBr + Ar free jets: Rotational relaxation of HBr, A.E. Belikov, M.M. Ahern and M.A. Smith 234 (1998) 195
- Vibrational modes in layered double hydroxides and their calcined derivatives, W. Kargunya, R. Baddour-Hadjean, F. Kooli and W. Jones 236 (1998) 225
- The B ← X spectrum of ArCl₂: linear and perpendicular isomers, K.C. Janda, D. Djahandideh, O. Roncero and N. Halberstadt 239 (1998) 177
- Large-amplitude motion in highly quantum clusters: high-resolution infrared absorption studies of jet-cooled H₂–HCl and H₂–DCI, D.T. Anderson, M. Schuder and D.J. Nesbitt 239 (1998) 253
- On librational broadening of vibrational transitions in liquids: a simple model, D.J. Ulness, J.C. Kirkwood and A.C. Albrecht 240 (1999) 109
- Molecular dynamics of many particle systems and condensed phases*
- Molecular relaxation in simple dipolar liquids confined between two solid surfaces, S. Senapati and A. Chandra 231 (1998) 65
- Effect of pressure and temperature on the H-atom tunneling in solid phase chemical reactions. The acridine/fluorene system, L.I. Trakhtenberg and V.L. Klochikhin 232 (1998) 175
- Molecular dynamics studies of NaCl solutions in methanol–water mixtures. An effect of NaCl on hydrogen bonded network, E. Hawlicka and D. Swiatla-Wojcik 232 (1998) 361
- Free energies of solvation for peptides and polypeptides using SCRF methods, C. Alemán, H.M. Ishiki, E.A. Armelin, O. Abrahão Junior and S.E. Galembeck 233 (1998) 85
- Quantum time correlation functions and classical coherence, R. Hernandez and G.A. Voth 233 (1998) 243
- A viscoelastic continuum model of non-polar solvation. II. Vibrational dephasing in moderate to high-viscosity liquids and glasses, M.A. Berg and H.W. Hubble 233 (1998) 257
- Heterodyne-detected stimulated photon echo: applications to optical dynamics in solution, W.P. de Boeij, M.S. Pshenichnikov and D.A. Wiersma 233 (1998) 287
- Dynamics of structural relaxation upon Rydberg excitation of an impurity in an Ar crystal, S. Jimenez, A. Pasquarello, R. Car and M. Chergui 233 (1998) 343
- Wavepacket diagnosis with chirped probe pulses, R. Zadoyan, N. Schwentner and V.A. Apkarian 233 (1998) 353
- The librational and vibrational spectra of water in natrolite, Na₂Al₂Si₃O₁₀ · 2H₂O compared with ab-initio calculations, C.M.B. Line and G.J. Kearley 234 (1998) 207

- Vibrational energy relaxation in liquid oxygen, K.F. Everitt, S.A. Egorov and J.L. Skinner 235 (1998) 115
- Effects of non-Markovian relaxation in the femtosecond differential absorption spectra, E. Gaižauskas, A. Beržanskis and K.-H. Feller 235 (1998) 123
- Numerical simulations of solvation in simple polar fluids: dependence on the thermodynamic state below and above the critical point, P. Graf and A. Nitzan 235 (1998) 297
- An intermolecular potential function for Na^+ -acetonitrile obtained from ab initio calculations. Application to liquid simulations, E.M. Cabaleiro-Lago and M.A. Ríos 236 (1998) 235
- Constant temperature simulations using the Langevin equation with velocity Verlet integration, M.G. Paterlini and D.M. Ferguson 236 (1998) 243
- Vibrational spectroscopy and molecular dynamics of solvated methanol tetramer and pentamer, D. Meyer zum Büschenfelde and A. Staib 236 (1998) 253
- Interference-effects in the laser-induced desorption of small molecules from surfaces: a model study, S. Thiel, T. Klüner and H.-J. Freund 236 (1998) 263
- The energy relaxation of Si-H vibration in the H/Si(111) system. Relaxation rate and potential energy surface anharmonicity, V.A. Ermoshin, A.K. Kazansky, K.S. Smirnov and D. Bougeard 237 (1998) 333
- Dielectric effects of step-increased pressure on the mass- and diffusion-controlled linear chain and network macromolecules growth, D.A. Wasylyshyn and G.P. Johari 237 (1998) 345
- On the use of evaporation dynamics to characterize phase transitions in van der Waals clusters: investigations in aniline-(argon) $_n$ up to $n = 15$, P. Parneix, F.G. Amar and P. Bréchnignac 239 (1998) 121
- Modeling structure and dynamics of solvated molecular ions: Photodissociation and recombination in $\text{I}_2^-(\text{CO}_2)_n$, J. Faeder, N. Delaney, P.E. Maslen and R. Parson 239 (1998) 525
- Effect of solvent fluctuations on proton transfer dynamics: a hybrid AM1/MM molecular dynamics simulation on the $[\text{H}_3\text{N}-\text{H}-\text{NH}_3]^+$ system, G.-S. Li, M.T.C. Martins Costa, C. Millot and M.F. Ruiz-López 240 (1999) 93
- On the nonequilibrium effects in thermally activated reactions $A + A \rightleftharpoons B + B \rightleftharpoons C + C$, J. Gorecki and J.N. Gorecka 240 (1999) 215
- Competition between electronic and vibrational predissociation in $\text{Ar}-\text{I}_2(B)$: a molecular dynamics with quantum transitions study, A. Bastida, J. Zuñiga, A. Requena, N. Halberstadt and J.A. Beswick 240 (1999) 229
- A semiclassical surface-hopping procedure for vibrational relaxation in polyatomic molecules: model calculations, P. Velez and M.F. Herman 240 (1999) 241
- Quasiparticle dynamics (incl. excitons, polarons)*
- Instability of self-trapped Frenkel exciton states in one-dimensional microcrystallites, M. Takeshima, J. Singh and A.H. Matsui 233 (1998) 97
- Electronic structure of planar superconducting systems. From finite to extended model, S. Larsson 236 (1998) 133
- Quantum motion of particles along one-dimensional pathways with static and dynamic energy disorder, L.D.A. Siebbeles and Y.A. Berlin 238 (1998) 97
- Simulation of excitonic optical line shapes of cyclic molecular aggregates with 9 and 18 units: influence of quasi-static and dynamic disorder, I. Barvák, C. Warns, T. Neidlinger and P. Reineker 240 (1999) 173
- Migration and interaction on grids and lattices*
- Quantum superconductor-metal transition in a 2D proximity-coupled array, M.V. Feigel'man and A.I. Larkin 235 (1998) 107

- Transport kinetics of triplet excitation in solid chrysene, S.A. Bagnich 237 (1998) 359
- Quantum motion of particles along one-dimensional pathways with static and dynamic energy disorder, L.D.A. Siebbeles and Y.A. Berlin 238 (1998) 97
- Yamanouchi-chain \mathcal{S}_n -invariant hierarchies for SR carrier space of $\{T^k(v)\}(SU2 \times \mathcal{S}_n)$ dual tensors in NMR: some maximal \mathcal{S}_n -inner products, via \mathcal{S}_n -restricted-space Schur Fn. product mappings, F.P. Temme 238 (1998) 245
- Nonequilibrium dissociation of hydrogen in a parallel-plate radio frequency discharge, S. Longo and I.D. Boyd 238 (1998) 445
- Statistical computational methods (incl. Monte Carlo)*
- Monte Carlo calculation of partition functions for straight chain alkanes, J. Gang, M.J. Pilling and S.H. Robertson 231 (1998) 183
- Bridged-assisted electron transfer. Random matrix theory approach, E. Gudowska-Nowak, G. Papp and J. Brickmann 232 (1998) 247
- Quantum hysteresis and resonant tunneling in bistable systems, M. Thorwart, P. Reimann, P. Jung and R.F. Fox 235 (1998) 61
- Numerical simulations of solvation in simple polar fluids: dependence on the thermodynamic state below and above the critical point, P. Graf and A. Nitzan 235 (1998) 297
- Modelling aluminium clusters with an empirical many-body potential, L.D. Lloyd and R.L. Johnston 236 (1998) 107
- An intermolecular potential function for Na^+ -acetonitrile obtained from ab initio calculations. Application to liquid simulations, E.M. Cabaleiro-Lago and M.A. Ríos 236 (1998) 235
- Hybrid procedure of the ab initio molecular orbital (MO) method and the Monte Carlo samplings; application to cluster $\text{B}^+(\text{H}_2\text{O})$, H. Watanabe and T. Asada 237 (1998) 81
- Nonequilibrium dissociation of hydrogen in a parallel-plate radio frequency discharge, S. Longo and I.D. Boyd 238 (1998) 445
- Existence of two internal energy distributions in jet-formed van der Waals heteroclusters: example of the anthracene-argon_n system, D. Uridat, V. Brenner, I. Dimicoli, J. Le Calvé, P. Millié, M. Mons and F. Piuze 239 (1998) 151
- Melting behavior of the $(\text{H}_2\text{O})_6$ and $(\text{H}_2\text{O})_8$ clusters, J.M. Pedulla and K.D. Jordan 239 (1998) 593
- Dynamics of structures, lattices and macromolecular conformations*
- Perylene in biphenyl and anthracene crystals: an example of the influence of the host on single-molecule signals, P.J. Walla, F. Jelezko, Ph. Tamarat, B. Lounis and M. Orrit 233 (1998) 117
- Constant temperature simulations using the Langevin equation with velocity Verlet integration, M.G. Paterlini and D.M. Ferguson 236 (1998) 243
- Fluctuations and random processes*
- Bridged-assisted electron transfer. Random matrix theory approach, E. Gudowska-Nowak, G. Papp and J. Brickmann 232 (1998) 247
- Population relaxation and non-Markovian frequency fluctuations in third- and fifth-order Raman scattering, T. Steffen and K. Duppen 233 (1998) 267
- Mathematical aspects of the fluctuating barrier problem. Existence of equilibrium and relaxation solutions, P. Pechukas and J. Ankerhold 235 (1998) 5
- Reaction rates when barriers fluctuate: A singular perturbation approach, P. Reimann, R. Bartussek and P. Hänggi 235 (1998) 11
- Brownian transport controlled by dichotomic and thermal fluctuations, J. Kula, M. Kostur and J. Łuczka 235 (1998) 27

- Thermal decay of a metastable elastic string, C. Cattuto, M. Borromeo and F. Marchesoni 235 (1998) 51
- Suppression of quantum coherence: Noise effect, J. Shao, C. Zerbe and P. Hänggi 235 (1998) 81
- Binary collision theory for thermal and nonisothermal relaxation and reaction of polyatomic molecules, P. Talkner, E. Pollak and A.M. Berezhkovskii 235 (1998) 131
- On the role of the energy loss in turnover theories of activated rate processes, A.N. Drozdov and J.J. Brey 235 (1998) 147
- The Kramers problem in 2D-coupled periodic potentials, G. Caratti, R. Ferrando, R. Spadacini and G.E. Tommei 235 (1998) 157
- Curvilinear-path based theory of the energy transfer limited rate of a two-dimensional solute in a dissipative bath, S.K. Reese and S.C. Tucker 235 (1998) 171
- Reversible chemical reactions in slowly relaxing environments: Kramers' turnover of the rate constant, A.M. Berezhkovskii, V.Yu. Zitserman, D.-Y. Yang and S.H. Lin 235 (1998) 201
- Where is the exit point?, Z. Schuss and A. Spivak 235 (1998) 227
- Non-equilibrium statistical mechanics*
- Molecular relaxation in simple dipolar liquids confined between two solid surfaces, S. Senapati and A. Chandra 231 (1998) 65
- Reaction rates when barriers fluctuate: A singular perturbation approach, P. Reimann, R. Bartussek and P. Hänggi 235 (1998) 11
- Thermodynamical and mechanical efficiency of a ratchet pump, I.M. Sokolov and A. Blumen 235 (1998) 39
- Thermal decay of a metastable elastic string, C. Cattuto, M. Borromeo and F. Marchesoni 235 (1998) 51
- Quantum hysteresis and resonant tunneling in bistable systems, M. Thorwart, P. Reimann, P. Jung and R.F. Fox 235 (1998) 61
- Binary collision theory for thermal and nonisothermal relaxation and reaction of polyatomic molecules, P. Talkner, E. Pollak and A.M. Berezhkovskii 235 (1998) 131
- On the role of the energy loss in turnover theories of activated rate processes, A.N. Drozdov and J.J. Brey 235 (1998) 147
- Saddle point avoidance due to inhomogeneous friction, G.J. Moro and F. Cardin 235 (1998) 189
- Reversible chemical reactions in slowly relaxing environments: Kramers' turnover of the rate constant, A.M. Berezhkovskii, V.Yu. Zitserman, D.-Y. Yang and S.H. Lin 235 (1998) 201
- Where is the exit point?, Z. Schuss and A. Spivak 235 (1998) 227
- Nonadiabatic reactions in condensed phase in the absence of thermal equilibrium, I. Rips 235 (1998) 243
- Numerical simulations of solvation in simple polar fluids: dependence on the thermodynamic state below and above the critical point, P. Graf and A. Nitzan 235 (1998) 297
- Analytical theory of time-resolved fluorescence anisotropy and dynamic Stokes shift of polar solute molecules based on continuum model for solvent, F. Tanaka and N. Mataga 236 (1998) 277
- On the dependence of a critical supersaturation on pressure of a two-component background gas in a diffusion cloud chamber, A.L. Itkin 238 (1998) 273
- Solvent effects on outersphere electron transfer reactions in mixed dipolar liquids, A. Chandra 238 (1998) 285
- Penning ionization of C_{60} and C_{70} , J.M. Weber, K. Hansen, M.-W. Ruf and H. Hotop 239 (1998) 271
- Effect of solvent fluctuations on proton transfer dynamics: a hybrid AM1/MM molecular dynamics simulation on the $[H_3N-H-NH_3]^+$ system, G.-S. Li, M.T.C. Martins Costa, C. Millot and M.F. Ruiz-López 240 (1999) 93
- Non-equilibrium thermodynamic and hydrodynamic theories*
- ^{13}C NMR relaxation in neutral and charged tetra-*n*-alkyl compounds, B. Bordes, F. Coletta, A. Ferrarini, F. Gottardi and P.L. Nordio 231 (1998) 51

- A frequency-resolved cavity model (FRCM) for treating equilibrium and non-equilibrium solvation energies, M.V. Basilevsky, I.V. Rostov and M.D. Newton 232 (1998) 189
- A frequency-resolved cavity model (FRCM) for treating equilibrium and non-equilibrium solvation energies. 2: Evaluation of solvent reorganization energies, M.D. Newton, M.V. Basilevsky and I.V. Rostov 232 (1998) 201
- Solvent effects on outersphere electron transfer reactions in mixed dipolar liquids, A. Chandra 238 (1998) 285
- On the nonequilibrium effects in thermally activated reactions $A + A \rightleftharpoons B + B \rightleftharpoons C + C$, J. Gorecki and J.N. Gorecka 240 (1999) 215
- Equilibrium statistical mechanics and thermodynamics*
- Monte Carlo calculation of partition functions for straight chain alkanes, J. Gang, M.J. Pilling and S.H. Robertson 231 (1998) 183
- Direct observation of the equilibrium between cyclohexenyl radicals, O_2 , and cyclohexenylperoxy radicals, R. Zils, S. Inomata, Y. Okunuki and N. Washida 231 (1998) 303
- Water anomalies and the double-well Takahashi model, C.H. Cho, S. Singh and G.W. Robinson 232 (1998) 329
- Electrical properties of a charged surface in a general electrolyte solution, Y.-C. Kuo and J.-P. Hsu 236 (1998) 1
- Constant temperature simulations using the Langevin equation with velocity Verlet integration, M.G. Paterlini and D.M. Ferguson 236 (1998) 243
- Vibrational spectroscopy and molecular dynamics of solvated methanol tetramer and pentamer, D. Meyer zum Büschenfelde and A. Staib 236 (1998) 253
- Melting behavior of the $(H_2O)_6$ and $(H_2O)_8$ clusters, J.M. Pedulla and K.D. Jordan 239 (1998) 593
- Extremum methods for ensembles (energy, entropy, free energy)*
- Cavitation contribution to the free energy of solvation. Comparison of different formalisms in the context of MST calculations, C. Colominas, F.J. Luque, J. Teixidó and M. Orozco 240 (1999) 253
- Theory of critical behavior*
- Thermal decay of a metastable elastic string, C. Cattuto, M. Borromeo and F. Marchesoni 235 (1998) 51
- Time and space correlation functions*
- Quantum time correlation functions and classical coherence, R. Hernandez and G.A. Voth 233 (1998) 243
- Heterodyne-detected stimulated photon echo: applications to optical dynamics in solution, W.P. de Boeij, M.S. Pshenichnikov and D.A. Wiersma 233 (1998) 287
- A diffusive model for interpreting solvation dynamics in isotropic and ordered liquid phases, A. Polimeno, G. Saielli and P.L. Nordio 235 (1998) 313
- A Keilson–Storer type collision kernel for rotation–translation coupling, M.F. Gelin 240 (1999) 265
- Experiment**
- Magnetic resonances*
- Differential ring proton NMR shieldings and cyclic stabilization energies, D.B. Chesnut 231 (1998) 1
- ^{13}C NMR relaxation in neutral and charged tetra-*n*-alkyl compounds, B. Bordes, F. Coletta, A. Ferrarini, F. Gottardi and P.L. Nordio 231 (1998) 51
- ^{17}O quadrupole coupling in $C-O-H \cdots O=C$ hydrogen bonds, J. Seliger 231 (1998) 81
- Solvent effects on NMR spectrum of acetylene calculated by ab initio methods, M. Pecul and J. Sadlej 234 (1998) 111

- ¹⁷O nuclear quadrupole resonance study of proton disorder in solid benzoic acid, 4-hydroxybenzoic acid and 4-nitrobenzoic acid, J. Seliger and V. Žagar 234 (1998) 223
- High frequency satellites in resonant activation, E. Turlot, S. Linkwitz, D. Esteve, C. Urbina, M.H. Devoret and H. Grabert 235 (1998) 47
- Isotope effect in diffusion of methyl radicals in glassy ethanol-1,2-*d*₅ at low temperatures, V.L. Vyazovkin and V.A. Tolkachev 236 (1998) 291
- Recognition and characterization of binding modes of Δ - and Λ -[Ru(phen)₃]²⁺ and Δ - and Λ -[Ru(phen)₂DPPZ]²⁺ by the ²³Na NMR relaxation and binding free energy parameters, F.C. Marincola, M. Casu, G. Saba, A. Lai, P. Lincoln and B. Nordén 236 (1998) 301
- Linear response calculations of electronic *g*-factors and spin-rotational coupling constants for diatomic molecules with a triplet ground state, M. Engström, B. Minaev, O. Vahtras and H. Ågren 237 (1998) 149
- Rotational tunneling of methyl groups in the hydroquinone/acetonitrile clathrate: A combined deuteron NMR, INS, and computational study, A. Detken, P. Schiebel, M.R. Johnson, H. Zimmermann and U. Haeberlen 238 (1998) 301
- 'Fractional heating' differential scanning calorimetry: a tool to study energetics and kinetics of solid-state reactions in photoactive systems with distributed parameters, J. Sworakowski and S. Nešpůrek 238 (1998) 343
- Electron paramagnetic resonance of Er³⁺ doped in YVO₄: hyperfine parameters, S.K. Misra, S. Isber, J.A. Capobianco and E. Cavalli 240 (1999) 313

Molecular spectroscopy

- High-resolution photoelectron spectroscopy using multibunch synchrotron radiation: rotational-resolved photoelectron bands of O₂⁺(b ⁴Σ_g[−], *v*⁺), C.-W. Hsu, M. Evans, S. Stimson, C.Y. Ng and P. Heimann 231 (1998) 121
- A theoretical study of the electronic structure and spectroscopic properties of the low-lying electronic states of the molecule AlSi, F.R. Ornellas and S. Iwata 232 (1998) 95
- Heterodyne-detected stimulated photon echo: applications to optical dynamics in solution, W.P. de Boeij, M.S. Pshenichnikov and D.A. Wiersma 233 (1998) 287
- Ab initio study of the X²Σ⁺ and A²Π states of the SiO⁺ cation including the effect of core correlation, Z.-L. Cai and J.P. François 234 (1998) 59
- Kinetics of the CN + CH₂CO and NCO + CH₂CO reactions, M.A. Edwards and J.F. Hershberger 234 (1998) 231
- Vibronic coupling effects in the low-energy 1²B_{1g} and 2²B_{1g} states of the C₁₀H₈⁺ radical, T. Andruniow and M. Pawlikowski 236 (1998) 35
- Vibrational modes in layered double hydroxides and their calcined derivatives, W. Kargunya, R. Baddour-Hadjean, F. Kooli and W. Jones 236 (1998) 225
- The structure of the lowest excited singlet (S₁) state of 4,4'-bipyridine: a picosecond time-resolved Raman analysis, C. Didierjean, V. De Waele, G. Buntinx and O. Poizat 237 (1998) 169
- Correlation corrected energy bands of nucleotide base stacks, F. Bogár and J. Ladik 237 (1998) 273
- Dielectric effects of step-increased pressure on the mass- and diffusion-controlled linear chain and network macromolecules growth, D.A. Wasylyshyn and G.P. Johari 237 (1998) 345
- Peculiarity of triplet-triplet energy transfer from 2-(2'-hydroxy-phenyl)benzoxazole to diacetyl. Evidence for radiative keto-enol transitions ³K* → ¹E and ¹E → ¹K*, B. Nickel and P.J. Walla 237 (1998) 371
- Ab initio study of the electronic spectrum of C₂H₂⁺. I. Vertical spectrum and angular potential curves, M. Perić, B. Engels and M. Hanrath 238 (1998) 33

- Ab initio study of the electronic spectrum of $C_2H_2^+$. II. Stretching potential energy surfaces for low-lying doublet electronic states, M. Perić and B. Engels 238 (1998) 47
- The first-order electric field-induced spectra: theory and experimental study of NO_2 , J.H. Chen, P.N. Wang, F.M. Li, Y.Q. Chen and Z.G. Wang 238 (1998) 165
- Wavelength dependence of the nonlinear absorption properties of laser dyes in solid and liquid solutions, J. Barroso, A. Costela, I. García-Moreno and R. Sastre 238 (1998) 257
- Manifestation of interaction of the transition dipole moments in IR spectra of low-temperature liquids and solutions in liquefied noble gases, T.D. Kolomiitsova, A.P. Burtsev, V.G. Fedoseev and D.N. Shchepkin 238 (1998) 315
- 'Fractional heating' differential scanning calorimetry: a tool to study energetics and kinetics of solid-state reactions in photoactive systems with distributed parameters, J. Sworakowski and S. Nešpůrek 238 (1998) 343
- Volume phase transition of polymer gel in water and heavy water, H. Shirota, N. Endo and K. Horie 238 (1998) 487
- Impedance spectroscopic investigation of the temperature influence on the transfer of tetraphenylborate ions through lipid membranes — Calculation of energy barriers for the ion transfer across lipid membranes, K.-D. Schulze 238 (1998) 495
- Hydrogen bonding in (substituted benzene) · (water)_n clusters with $n \leq 4$, H.-D. Barth, K. Buchhold, S. Djafari, B. Reimann, U. Lommatzsch and B. Brutschy 239 (1998) 49
- Equatorial piperidine and the piperidine–water complex. Rotational spectra and molecular structures, U. Spoerel and W. Stahl 239 (1998) 97
- Laser-induced fluorescence spectroscopy of van der Waals complexes of tetracene– Ar_N ($N \leq 5$) and pentacene–Ar within ultracold liquid He droplets, M. Hartmann, A. Lindinger, J.P. Toennies and A.F. Vilesov 239 (1998) 139
- A contribution to the structure determination of Ar–thiophene: the electric dipole moment, U. Spoerel and D. Consalvo 239 (1998) 199
- Photodissociation spectroscopy of (benzene–toluene)⁺. Charge delocalization in the hetero-dimer ion, K. Ohashi, Y. Nakane, Y. Inokuchi, Y. Nakai and N. Nishi 239 (1998) 429
- Photoelectron–photofragment coincidence studies of the dissociative photodetachment of O_4^- , K.A. Hanold and R.E. Continetti 239 (1998) 493
- Infrared absorption and Raman scattering of (Z)-3-hydroxypropenal. A density functional theoretical study, J. Spanget-Larsen 240 (1999) 51
- A gas phase ab initio excited state geometry optimization study of thymine, cytosine and uracil, M.K. Shukla and P.C. Mishra 240 (1999) 319
- Are the changes in the lifetime of the excited uranyl ion of chemical or physical nature?, M. Bouby, I. Billard, A. Bonnenfant and G. Klein 240 (1999) 353
- microwave*
- Rotational spectra of the ^{15}N -aniline–X, (X = Ar, Ne) complexes. Structure determination from studies on isotopomers, V. Storm, H. Dreizler and D. Consalvo 237 (1998) 395
- Equatorial piperidine and the piperidine–water complex. Rotational spectra and molecular structures, U. Spoerel and W. Stahl 239 (1998) 97
- A contribution to the rotational spectrum, structure, and dynamics of the benzonitrile–water complex in the S_0 electronic state, V. Storm, H. Dreizler and D. Consalvo 239 (1998) 109
- A contribution to the structure determination of Ar–thiophene: the electric dipole moment, U. Spoerel and D. Consalvo 239 (1998) 199
- Adducts of aromatic molecules with rare gases: rotational spectrum of pyrazole–argon, W. Caminati, P.G. Favero and B. Velino 239 (1998) 223

- Rotational spectrum and dynamics of tetrahydrofuran–argon, S. Melandri, J.C. López, P.G. Favero, W. Caminati and J.L. Alonso 239 (1998) 229
- Electric field effect on the upper critical solution temperature, K. Orzechowski 240 (1999) 275
- infrared*
- Infrared spectroscopy of the NO₃ radical, K. Kawaguchi, T. Ishiwata, E. Hirota and I. Tanaka 231 (1998) 193
- Mode-dependent anharmonic coupling between OH stretching and intermolecular vibrations of the hydrogen-bonded clusters of phenol, T. Ebata, K. Nagao and N. Mikami 231 (1998) 199
- New results on the atmospheric photooxidation of simple alkylbenzenes, B. Klotz, I. Barnes and K.H. Becker 231 (1998) 289
- The vibrational spectroscopy of C₆₀H₃₆: An experimental and theoretical study, R. Bini, J. Ebenhoch, M. Fanti, P.W. Fowler, S. Leach, G. Orlandi, Ch. Rüchardt, J.P.B. Sandall and F. Zerbetto 232 (1998) 75
- Ultrafast laser control of vibrational dynamics for a two-dimensional model of HONO₂ in the ground electronic state: separation of conformers, control of the bond length, selective preparation of the discrete and the continuum states, M. Oppel and G.K. Paramonov 232 (1998) 111
- Model study of proton transfer in a H-bonded cluster with an A–H...B reaction complex. Introduction of an effective coordinate for the solvation shell, M.V. Vener 233 (1998) 77
- Controlling condensed-phase vibrational excitation with tailored infrared pulses, V.D. Kleiman, S.M. Arrivo, J.S. Melinger and E.J. Heilweil 233 (1998) 207
- The librational and vibrational spectra of water in natrolite, Na₂Al₂Si₃O₁₀ · 2H₂O compared with ab-initio calculations, C.M.B. Line and G.J. Kearley 234 (1998) 207
- Kinetics of the CN + CH₂CO and NCO + CH₂CO reactions, M.A. Edwards and J.F. Hersberger 234 (1998) 231
- Matrix photochemistry of nitrosyl chloride. Interconversion of ClNO and ClON species by irradiation and tunneling effect, A. Hallou, L. Schriver-Mazzuoli, A. Schriver and P. Chaquin 237 (1998) 251
- Infrared spectra and theoretical calculations of HCl complexed with NO, L. Krim and M.E. Alikhani 237 (1998) 265
- IR–IR double-resonance studies of vibrational relaxation of CD₃F in solid and liquid Xe, Kr, Ar solutions near the melting point, K.S. Rutkowski 237 (1998) 403
- On the dielectric continuum solvent model for theoretical estimates of the conformational equilibrium of molecules with an intramolecular hydrogen bond, T. Yasuda and S.-i. Ikawa 238 (1998) 173
- Vibrational analysis of 2-nitrophenol. A joint FT-IR, FT-Raman and scaled quantum mechanical study, A. Kovács, V. Izvekov, G. Keresztury and G. Pongor 238 (1998) 231
- Manifestation of interaction of the transition dipole moments in IR spectra of low-temperature liquids and solutions in liquefied noble gases, T.D. Kolomiitsova, A.P. Burtsev, V.G. Fedoseev and D.N. Shchepkin 238 (1998) 315
- Vibrational spectroscopy of single methanol molecules attached to liquid water clusters, F. Huisken, S. Mohammad-Pooran and O. Werhahn 239 (1998) 11
- Hydrogen bonding in (substituted benzene) · (water)_n clusters with $n \leq 4$, H.-D. Barth, K. Buchhold, S. Djafari, B. Reimann, U. Lommatzsch and B. Brutschy 239 (1998) 49
- Resonant ion-dip infrared spectroscopy of benzene–(water)_n–(methanol)_m clusters with $n + m = 4, 5$, F.C. Hagemeister, C.J. Gruenloh and T.S. Zwier 239 (1998) 83

- Large-amplitude motion in highly quantum clusters: high-resolution infrared absorption studies of jet-cooled $\text{H}_2\text{--HCl}$ and $\text{H}_2\text{--DCI}$, D.T. Anderson, M. Schuder and D.J. Nesbitt 239 (1998) 253
- Mode dependence of the state-to-state vibrational dynamics of HCN--HF , L. Oudejans and R.E. Miller 239 (1998) 345
- Vibrational and unimolecular dissociation of mixed solvent cluster ions: $\text{Na}^+(\text{CH}_3)_2\text{CO})_n(\text{CH}_3\text{OH})_m$, C.J. Weinheimer and J.M. Lisy 239 (1998) 357
- Infrared photodissociation spectra of isomeric $\text{SiOH}^+\text{--Ar}_n$ ($n = 1\text{--}10$) complexes, R.V. Olkhov, S.A. Nizkorodov and O. Dopfer 239 (1998) 393
- Mass-selected "matrix isolation" infrared spectroscopy of the $\text{I}^-\cdot(\text{H}_2\text{O})_2$ complex: making and breaking the inter-water hydrogen-bond, P. Ayotte, G.H. Weddle, J. Kim and M.A. Johnson 239 (1998) 485
- Raman**
- The vibrational spectroscopy of $\text{C}_{60}\text{H}_{36}$: An experimental and theoretical study, R. Bini, J. Ebenhoch, M. Fanti, P.W. Fowler, S. Leach, G. Orlandi, Ch. Rüchardt, J.P.B. Sandall and F. Zerbetto 232 (1998) 75
- Populations of rotational levels of nitrogen molecules in free jets. Comparison of CARS and electron beam fluorescent technique, R.G. Sharafutdinov, A.A. Ilyukhin, V.V. Smirnov, A.E. Belikov, G.I. Sukhinin and R.L. Pykhov 233 (1998) 127
- The intermolecular interaction mechanisms in liquid CS_2 at 295 and 165 K probed with two-dimensional Raman spectroscopy, A. Tokmakoff, M.J. Lang, X.J. Jordanides and G.R. Fleming 233 (1998) 231
- A viscoelastic continuum model of non-polar solvation. II. Vibrational dephasing in moderate to high-viscosity liquids and glasses, M.A. Berg and H.W. Hubble 233 (1998) 257
- Population relaxation and non-Markovian frequency fluctuations in third- and fifth-order Raman scattering, T. Steffen and K. Duppen 233 (1998) 267
- Time-resolved resonance Raman and molecular orbital studies of charge separation and intramolecular reorganisation, G.D. Scholes, I.R. Gould, A.W. Parker and D. Phillips 234 (1998) 21
- CARS studies of bending states of CO_2 : evidence of collisional rotational transitions with odd ΔJ , A.P. Kouzov, D.N. Kozlov and B. Hemmerling 236 (1998) 15
- Franck–Condon effects in low-energy states of $\text{C}_{10}\text{H}_8^+$ radical. Ab initio MCSCF study of absorption and resonance Raman spectra, T. Andruniow and M. Pawlikowski 236 (1998) 25
- Sub-picosecond excited-state dynamics of a carotenoid (spirilloxanthin) in the light-harvesting systems of *Chromatium vinosum*. Relaxation process from the optically allowed S_2 state, H. Okamoto, M. Ogura, T. Nakabayashi and M. Tasumi 236 (1998) 309
- The structure of the lowest excited singlet (S_1) state of 4,4'-bipyridine: a picosecond time-resolved Raman analysis, C. Didierjean, V. De Waele, G. Buntinx and O. Poizat 237 (1998) 169
- Vibrational analysis of 2-nitrophenol. A joint FT-IR, FT-Raman and scaled quantum mechanical study, A. Kovács, V. Izvekov, G. Keresztury and G. Pongor 238 (1998) 231
- Raman spectroscopy study on the dynamic behavior of nitrate anion in zinc nitrate solution at high temperatures and pressure, Y. Ikushima and M. Arai 238 (1998) 455
- ZEKE electron spectroscopy of azulene and azulene–argon, D. Tanaka, S. Sato and K. Kimura 239 (1998) 437
- UV**
- Photochemistry of acetone under tropospheric conditions, T. Gierczak, J.B. Burkholder, S. Bauerle and A.R. Ravishankara 231 (1998) 229

- On the UV photodissociation dynamics of hydrogen iodide, S.R. Langford, P.M. Regan, A.J. Orr-Ewing and M.N.R. Ashfold 231 (1998) 245
- Electronic spectroscopy and predissociation mechanism of Ar–NO in the 3p Rydberg states, K. Tsuji, K. Aiuchi, K. Shibuya and K. Obi 231 (1998) 279
- Fluorescence lifetime of rovibrational states of h_4 -acetaldehyde and spectra of d_4 -acetaldehyde, S.-H. Jen, T.-J. Hsu and I.-C. Chen 232 (1998) 131
- Femtosecond photodissociation of triiodide in solution: Excitation energy dependence and transition state dynamics, T. Kühne, R. Küster and P. Vöhringer 233 (1998) 161
- Light induced *cis*–*trans* isomerization of azo compounds in polymethyl methacrylate, S.Yu. Grebenkin and B.V. Bol'shakov 234 (1998) 239
- Vibronic coupling effects in the low-energy 1^2B_{1g} and 2^2B_{1g} states of the $\text{C}_{10}\text{H}_8^+$ radical, T. Andruniow and M. Pawlikowski 236 (1998) 35
- Ultraviolet absorption spectrum and cross-sections of vinyl (C_2H_3) radical in the 225–238 nm region, A. Fahr, P. Hassanzadeh and D.B. Atkinson 236 (1998) 43
- Interference-effects in the laser-induced desorption of small molecules from surfaces: a model study, S. Thiel, T. Klüner and H.-J. Freund 236 (1998) 263
- Emission spectra of HeAr_2^+ and HeKr_2^+ heterotrimer ions produced in a helium flowing afterglow, M. Tsuji, M. Tanaka, E. Oda, H. Ishimi and Y. Nishimura 236 (1998) 319
- Correlation corrected energy bands of nucleotide base stacks, F. Bogár and J. Ladik 237 (1998) 273
- Proximity effects in the excited state ordering and photophysics of thienyl-pyridyl ketones, A. Romani, F. Ortica and G. Favaro 237 (1998) 413
- Complexes of spiropyran-derived merocyanines with metal ions: relaxation kinetics, photochemistry and solvent effects, A.K. Chibisov and H. Görner 237 (1998) 425
- On the electronic spectroscopy of benzyl alcohol, J.M. Gingell, G. Marston, N.J. Mason, H. Zhao and M.R.F. Siggel 237 (1998) 443
- The electronic states of pyrrole studied by optical (VUV) absorption, near-threshold electron energy-loss (EEL) spectroscopy and ab initio multi-reference configuration interaction calculations, M.H. Palmer, I.C. Walker and M.F. Guest 238 (1998) 179
- Double resonance spectroscopy of phenol(H_2O) $_{1-12}$: evidence for ice-like structures in aromate–water clusters?, W. Roth, M. Schmitt, Ch. Jacoby, D. Spangenberg, Ch. Janzen and K. Kleinermanns 239 (1998) 1
- Investigations of OH–N- and NH–O-type hydrogen-bonded clusters by UV laser spectroscopy, C. Jacoby, P. Hering, M. Schmitt, W. Roth and K. Kleinermanns 239 (1998) 23
- Highly resolved UV spectroscopy of clusters: isotope substitution studies of hydrogen-bonded phenol · water, R.M. Helm and H.J. Neusser 239 (1998) 33
- Electronic spectroscopy of jet-cooled anthracene/(H_2O) $_n$ clusters ($n = 1-16$): comparisons of inhomogeneous structure, P.M. Palmer and M.R. Topp 239 (1998) 65
- Resonant ion-dip infrared spectroscopy of benzene–(water) $_n$ –(methanol) $_m$ clusters with $n + m = 4, 5$, F.C. Hagemeister, C.J. Gruenloh and T.S. Zwier 239 (1998) 83
- Existence of two internal energy distributions in jet-formed van der Waals heteroclusters: example of the anthracene–argon $_n$ system, D. Uridat, V. Brenner, I. Dimicoli, J. Le Calvé, P. Millié, M. Mons and F. Piuze 239 (1998) 151
- Photodissociation of Mg^+ –(CH_3OH) $_N$ complexes: evidence for the onset of solvation, M.R. France, S.H. Pullins and M.A. Duncan 239 (1998) 447
- A gas phase ab initio excited state geometry optimization study of thymine, cytosine and uracil, M.K. Shukla and P.C. Mishra 240 (1999) 319
- Dual fluorescence of the isoquinolinium cation in methanol: time-resolved emission spectra and semiempirical calculations, A.D. Welland, F.W. Schneider and A.B.J. Parusel 240 (1999) 403

-visible

- Perylene in biphenyl and anthracene crystals: an example of the influence of the host on single-molecule signals, P.J. Walla, F. Jelezko, Ph. Tamarat, B. Lounis and M. Orrit 233 (1998) 117
- Time-resolved resonance Raman and molecular orbital studies of charge separation and intramolecular reorganisation, G.D. Scholes, I.R. Gould, A.W. Parker and D. Phillips 234 (1998) 21
- Kinetics of the $\text{CN} + \text{CH}_2\text{CO}$ and $\text{NCO} + \text{CH}_2\text{CO}$ reactions, M.A. Edwards and J.F. Hershberger 234 (1998) 231
- Vibronic coupling effects in the low-energy 1^2B_{1g} and 2^2B_{1g} states of the $\text{C}_{10}\text{H}_8^+$ radical, T. Andruniow and M. Pawlikowski 236 (1998) 35
- Emission spectra of HeAr_2^+ and HeKr_2^+ heterotrimer ions produced in a helium flowing afterglow, M. Tsuji, M. Tanaka, E. Oda, H. Ishimi and Y. Nishimura 236 (1998) 319
- Photophysical and lasing properties of pyrromethene 567 dye in liquid solution. Environment effects, F. López Arbeloa, T. López Arbeloa, I. López Arbeloa, I. García-Moreno, A. Costela, R. Sastre and F. Amat-Guerri 236 (1998) 331
- On the electronic energy disposal of calcium excited atom reactions with halogen-containing compounds: Electronic branching ratio and spin-orbit state populations, M. Garay, C.A. Rinaldi, J.M. Orea and A. González Ureña 236 (1998) 343
- Modelling the substitution effects of several rhodium(III) transition metal complexes using the angular overlap model, B. Gilliams, D. Vandenbroucke and C. Görrler-Walrand 237 (1998) 91
- Dramatic reduction in fluorescence quantum yield in mutants of Green Fluorescent Protein due to fast internal conversion, A.D. Kummer, C. Kompa, H. Lossau, F. Pöllinger-Dammer, M.E. Michel-Beyerle, C.M. Silva, E.J. Bylina, W.J. Coleman, M.M. Yang and D.C. Youvan 237 (1998) 183
- Transport kinetics of triplet excitation in solid chrysene, S.A. Bagnich 237 (1998) 359
- Proximity effects in the excited state ordering and photophysics of thienyl-pyridyl ketones, A. Romani, F. Ortica and G. Favaro 237 (1998) 413
- Complexes of spiropyran-derived merocyanines with metal ions: relaxation kinetics, photochemistry and solvent effects, A.K. Chibisov and H. Görner 237 (1998) 425
- Multi-photon dissociation of CHBr_3 at 248 and 193 nm: observation of the electronically excited $\text{CH}(\text{A}^2\Delta)$ product, J. Lindner, K. Ermisch and R. Wilhelm 238 (1998) 329
- 'Anomalous' density of states and rotational selection rules of loosely bound states of NO_2 , A. Delon, S. Heilliette and R. Jost 238 (1998) 465
- Ab initio theoretical optical rotations of small molecules, P.L. Polavarapu and D.K. Chakraborty 240 (1999) 1
- Dual fluorescence of the isoquinolinium cation in methanol: time-resolved emission spectra and semiempirical calculations, A.D. Welland, F.W. Schneider and A.B.J. Parusel 240 (1999) 403

Photon counting and phase fluorimetry

- Kinetic and mechanistic study of the reaction of atomic chlorine with methyl bromide over an extended temperature range, C.A. Piety, R. Soller, J.M. Nicovich, M.L. McKee and P.H. Wine 231 (1998) 155
- Dual fluorescence of the isoquinolinium cation in methanol: time-resolved emission spectra and semiempirical calculations, A.D. Welland, F.W. Schneider and A.B.J. Parusel 240 (1999) 403

Photoelectron and Auger spectroscopy

- High-resolution photoelectron spectroscopy using multibunch synchrotron radiation: rotational-resolved photoelectron bands of $\text{O}_2^+(\text{b}^4\Sigma_g^-, \nu^+)$, C.-W. Hsu, M. Evans, S. Stimson, C.Y. Ng and P. Heimann 231 (1998) 121

- A He(I) photoelectron spectroscopic study of the $\tilde{X}^2A''_2$ state of NH_3^+ and ND_3^+ . A reanalysis and evidence for the coriolis coupling between the bending ν_2 and ν_4 modes, R. Locht, B. Leyh, K. Hottmann and H. Baumgärtel 233 (1998) 145
- Investigation of the CS_2^{2+} dication using threshold photoelectrons coincidence spectroscopy, M. Hochlaf, R.I. Hall, F. Penent, J.H.D. Eland and P. Lablanquie 234 (1998) 249
- Dissociative photoionisation of NO_2 up to 26 eV, J.H.D. Eland and L. Karlsson 237 (1998) 139
- An experimental study of the valence shell photoelectron spectrum of the NO_2 molecule, P. Baltzer, L. Karlsson, B. Wannberg, D.M.P. Holland, M.A. MacDonald, M.A. Hayes and J.H.D. Eland 237 (1998) 451
- Complete basis set limit ionization potentials of O_3 and NO_2 using the multiconfigurational spin tensor electron propagator method (MCSTEP), A.J. McKellar, D. Heryadi, D.L. Yeager and J.A. Nichols 238 (1998) 1
- Vertical double ionization of the sulphur dioxide molecule, I.W. Griffiths, D.E. Parry and F.M. Harris 238 (1998) 21
- Reactivity of vinyl chloride ionic clusters, S. Martrenchard, C. Dedonder-Lardeux, I. Dimicoli, G. Grégoire, C. Jouvet, M. Mons and D. Solgadi 239 (1998) 331
- Structure and dynamics of the phenol–water–argon cation radical, D.M. Chapman, F.J. Hompf, K. Müller-Dethlefs, E. Waterstradt, P. Hobza and V. Špirko 239 (1998) 417
- Anion spectroscopy of uracil, thymine and the amino-oxo and amino-hydroxy tautomers of cytosine and their water clusters, J. Schiedt, R. Weinkauff, D.M. Neumark and E.W. Schlag 239 (1998) 511
- Multiphoton ionization*
- Spin-forbidden dissociation of ozone in the Huggins bands, W. Denzer, G. Hancock, J.C. Pinot de Moira and P.L. Tyley 231 (1998) 109
- Coulomb explosion dynamics of N_2 in intense laser field by mass-resolved momentum imaging, A. Hishikawa, A. Iwamae, K. Hoshina, M. Kono and K. Yamanouchi 231 (1998) 315
- Spin–orbit branching in the predissociation of the $C^1\Pi$ state of HCl and DCl: a manifestation of quantum interference, M.H. Alexander, X. Li, R. Liyanage and R.J. Gordon 231 (1998) 331
- C–Br bond rupture in 193 nm photodissociation of vinyl bromide, H. Katayanagi, N. Yonekura and T. Suzuki 231 (1998) 345
- Laser photodissociation of ketene at 230 nm, M. Castillejo, S. Couris, E. Lane, M. Martin and J. Ruiz 232 (1998) 353
- Mechanism of the coherent control of the photoionization and photodissociation of HI and DI, J.A. Fiss, L. Zhu, K. Suto, G. He and R.J. Gordon 233 (1998) 335
- REMPI spectroscopy of internal state populations in $HBr + Ar$ free jets: Rotational relaxation of HBr, A.E. Belikov, M.M. Ahern and M.A. Smith 234 (1998) 195
- Double resonance spectroscopy of phenol(H_2O) $_{1-12}$: evidence for ice-like structures in aromate–water clusters?, W. Roth, M. Schmitt, Ch. Jacoby, D. Spangenberg, Ch. Janzen and K. Kleinermanns 239 (1998) 1
- Investigations of OH–N- and NH–O-type hydrogen-bonded clusters by UV laser spectroscopy, C. Jacoby, P. Hering, M. Schmitt, W. Roth and K. Kleinermanns 239 (1998) 23
- Highly resolved UV spectroscopy of clusters: isotope substitution studies of hydrogen-bonded phenol · water, R.M. Helm and H.J. Neusser 239 (1998) 33
- Resonant ion-dip infrared spectroscopy of benzene–(water) $_n$ –(methanol) $_m$ clusters with $n + m = 4, 5$, F.C. Hagemeister, C.J. Gruenloh and T.S. Zwier 239 (1998) 83

- Charge stripping effects from highly charged iodine ions formed from Coulomb explosion of CH_3I clusters, L. Poth, Q. Zhong, J.V. Ford, S.M. Hurley and A.W. Castleman Jr. 239 (1998) 309
- Ultrafast dynamics of transition metal carbonyls. II. Picosecond evaporation after photodissociation of $\text{Cr}(\text{CO})_6 \cdot (\text{CH}_3\text{OH})_n$ heteroclusters at 280 nm, M. Gutmann, J.M. Janello and M.S. Dickebohm 239 (1998) 317
- Structure and dynamics of the phenol–water–argon cation radical, D.M. Chapman, F.J. Hompf, K. Müller-Dethlefs, E. Waterstradt, P. Hobza and V. Špirko 239 (1998) 417
- X-ray spectroscopy*
- On the electronic structure of Cu(III) and Ni(III) in $\text{La}_2\text{Li}_{1/2}\text{Cu}_{1/2}\text{O}_4$, $\text{Nd}_2\text{Li}_{1/2}\text{Ni}_{1/2}\text{O}_4$, and Cs_2KCuF_6 , Z. Hu, G. Kaindl, S.A. Warda, D. Reinen, F.M.F. de Groot and B.G. Müller 232 (1998) 63
- The electronic structure of poly(pyridine-2,5-diyl) investigated by soft X-ray absorption and emission spectroscopies, M. Magnuson, L. Yang, J.-H. Guo, C. Sâthe, A. Agui, J. Nordgren, Y. Luo, H. Ågren, N. Johansson, W.R. Salaneck, L.E. Horsburgh and A.P. Monkman 237 (1998) 295
- An X-ray absorption near edge spectroscopy (XANES) study on organochromium complexes at the Cr K-edge, C. Engemann, J. Hormes, A. Longen and K.H. Dötz 237 (1998) 471
- Electron impact spectroscopy*
- Quantitative studies of the photoabsorption (4.5–488 eV) and photoionization (9–59.5 eV) of methyl iodide using dipole electron impact techniques, T.N. Olney, G. Cooper and C.E. Brion 232 (1998) 211
- Populations of rotational levels of nitrogen molecules in free jets. Comparison of CARS and electron beam fluorescent technique, R.G. Sharafutdinov, A.A. Ilyukhin, V.V. Smirnov, A.E. Belikov, G.I. Sukhinin and R.L. Pykhov 233 (1998) 127
- On the electronic spectroscopy of benzyl alcohol, J.M. Gingell, G. Marston, N.J. Mason, H. Zhao and M.R.F. Siggel 237 (1998) 443
- Experimental and theoretical studies of the low-lying electronic states of the simplest benzylic amide [2]catenane, A.M. Brouwer, W.J. Buma, R. Caudano, M. Fanti, C.-A. Fustin, D.A. Leigh, A. Murphy, P. Rudolf, F. Zerbetto and J.M. Zwiier 238 (1998) 421
- High-resolution electron ionization study of CO , $(\text{CO})_2$ and $(\text{CO})_3$: appearance energies and bond dissociation energies, D. Muigg, G. Denifl, A. Stamatovic, O. Echt and T.D. Märk 239 (1998) 409
- Vibrational excitation of the $\text{C}^3\Pi_u$ state of N_2 by electron impact, G. Poparić, M. Vičić and D.S. Belić 240 (1999) 283
- Absolute photoabsorption oscillator strengths by electron energy loss methods: the valence and S 2p and 2s inner shells of sulphur dioxide in the discrete and continuum regions (3.5–260 eV), R. Feng, G. Cooper, G.R. Burton, C.E. Brion and L. Avaldi 240 (1999) 371
- Laser induced fluorescence*
- Reactions of $\text{N}_2^+(v)$ with CO and NO at thermal energy, M.J. Frost, S. Kato, V.M. Bierbaum and S.R. Leone 231 (1998) 145
- Translational energy and angular distributions of $\text{O}(^1\text{D})$ and $\text{O}(^3\text{P}_j)$ fragments in the UV photodissociation of ozone, K. Takahashi, N. Taniguchi, Y. Matsumi and M. Kawasaki 231 (1998) 171
- Mode-dependent anharmonic coupling between OH stretching and intermolecular vibrations of the hydrogen-bonded clusters of phenol, T. Ebata, K. Nagao and N. Mikami 231 (1998) 199

- Intramolecular proton-transfer cycle of 2,4-dimethoxy-6-(1-hydroxy-2-naphthyl)-s-triazine studied by laser photolysis, M. Moriyama, Y. Kawakami, S. Tobita and H. Shizuka 231 (1998) 205
- Uptake coefficient of OH radical on aqueous surface, A. Takami, S. Kato, A. Shimono and S. Koda 231 (1998) 215
- Fluorescence lifetime of rovibrational states of h_4 -acetaldehyde and spectra of d_4 -acetaldehyde, S.-H. Jen, T.-J. Hsu and I.-C. Chen 232 (1998) 131
- Polarisation effects in electronically inelastic collisions: $\text{SiFC}^2\Delta + \text{H}_2 \rightarrow \text{SiFB}^2\Sigma^+ + \text{H}_2$, N.A. Jackson, C.J. Randall and K.G. McKendrick 233 (1998) 45
- Ab initio calculations and supersonic jet studies on the geometry of 4-dimethylamino-benzonitrile (DMABN) and related compounds in the ground and excited state, U. Lommatzsch and B. Brutschy 234 (1998) 35
- REMPI spectroscopy of internal state populations in $\text{HBr} + \text{Ar}$ free jets: Rotational relaxation of HBr, A.E. Belikov, M.M. Ahern and M.A. Smith 234 (1998) 195
- Dramatic reduction in fluorescence quantum yield in mutants of Green Fluorescent Protein due to fast internal conversion, A.D. Kummer, C. Kompa, H. Lossau, F. Pöllinger-Dammer, M.E. Michel-Beyerle, C.M. Silva, E.J. Bylina, W.J. Coleman, M.M. Yang and D.C. Youvan 237 (1998) 183
- Reactions of $\text{C}(^1\text{D})$ with H_2 , HD and D_2 : kinetic isotope effect and the CD/CH branching ratio, K. Sato, N. Ishida, T. Kurakata, A. Iwasaki and S. Tsunashima 237 (1998) 195
- Rotational relaxation of perylene in *n*-alcohols and *n*-alkanes studied by two-photon-induced anisotropy decay, S.W. Pauls, J.F. Hedstrom and C.K. Johnson 237 (1998) 205
- Laser-induced fluorescence spectroscopy of van der Waals complexes of tetracene- Ar_N ($N \leq 5$) and pentacene-Ar within ultracold liquid He droplets, M. Hartmann, A. Lindinger, J.P. Toennies and A.F. Vilesov 239 (1998) 139
- Electronic spectroscopy and excited state dynamics of the $\text{Al}-\text{N}_2$ complex, X. Yang, I. Gerasimov and P.J. Dagdigan 239 (1998) 207
- Isomeric structures, large amplitude intermolecular motions and electronic relaxation of the propynal-Ar complex, P. DeRose, P.-Y. Cheng, B. Xue, S.-S. Ju and H.-L. Dai 239 (1998) 235
- Are the changes in the lifetime of the excited uranyl ion of chemical or physical nature?, M. Bouby, I. Billard, A. Bonnenfant and G. Klein 240 (1999) 353
- Comparative study of the spectroscopic properties of Cr^{4+} -doped LiAlO_2 and LiGaO_2 , S. Kück and S. Hartung 240 (1999) 387

Ultrafast measurements

- Optical limiting properties of a zinc porphyrin polymer and its dimer and monomer model compounds, F.M. Qureshi, S.J. Martin, X. Long, D.D.C. Bradley, F.Z. Henari, W.J. Blau, E.C. Smith, C.H. Wang, A.K. Kar and H.L. Anderson 231 (1998) 87
- Pathway approach to ultrafast photochemistry: potential surfaces, conical intersections and isomerizations of small polyenes, W. Fuß, S. Lochbrunner, A.M. Müller, T. Schikarski, W.E. Schmid and S.A. Trushin 232 (1998) 161
- Vibrational energy transfer processes in dye molecules after ultrafast excitation of skeletal modes, T. Dahinten, J. Baier and A. Seilmeier 232 (1998) 239
- Vibrational coherence in bacterial reaction centers: spectroscopic characterisation of motions active during primary electron transfer, M.H. Vos, M.R. Jones and J.-L. Martin 233 (1998) 179
- Vibrational coherence in ultrafast electron-transfer dynamics of oxazine 1 in *N,N*-dimethylaniline: simulation of a femtosecond pump-probe experiment, B. Wolfseder, L. Seidner, W. Domcke, G. Stock, M. Seel, S. Engleitner and W. Zinth 233 (1998) 323

- Wavepacket diagnosis with chirped probe pulses, R. Zadoyan, N. Schwentner and V.A. Apkarian 233 (1998) 353
- Time-resolved resonance Raman and molecular orbital studies of charge separation and intramolecular reorganisation, G.D. Scholes, I.R. Gould, A.W. Parker and D. Phillips 234 (1998) 21
- Photochemical accumulation and recombination of ion pairs undergoing the singlet–triplet conversion, A.I. Burshtein and A.Yu. Sivachenko 235 (1998) 257
- Femtosecond pump–probe studies of chlorine dioxide photochemistry in water and acetonitrile, M.J. Philpott, S.C. Hayes and P.J. Reid 236 (1998) 207
- Analytical theory of time-resolved fluorescence anisotropy and dynamic Stokes shift of polar solute molecules based on continuum model for solvent, F. Tanaka and N. Mataga 236 (1998) 277
- Sub-picosecond excited-state dynamics of a carotenoid (spirilloxanthin) in the light-harvesting systems of *Chromatium vinosum*. Relaxation process from the optically allowed S₂ state, H. Okamoto, M. Ogura, T. Nakabayashi and M. Tasumi 236 (1998) 309
- Ultrafast intermolecular electron transfer in coumarin–hydrazine system, H. Shirota, H. Pal, K. Tominaga and K. Yoshihara 236 (1998) 355
- Rotational relaxation of perylene in *n*-alcohols and *n*-alkanes studied by two-photon-induced anisotropy decay, S.W. Pauls, J.F. Hedstrom and C.K. Johnson 237 (1998) 205
- Ultrafast dynamics of transition metal carbonyls. II. Picosecond evaporation after photodissociation of Cr(CO)₆ · (CH₃OH)_{*n*} heteroclusters at 280 nm, M. Gutmann, J.M. Janello and M.S. Dickebohm 239 (1998) 317
- Nonlinear optics and spectroscopy*
- Optical limiting properties of a zinc porphyrin polymer and its dimer and monomer model compounds, F.M. Qureshi, S.J. Martin, X. Long, D.D.C. Bradley, F.Z. Henari, W.J. Blau, E.C. Smith, C.H. Wang, A.K. Kar and H.L. Anderson 231 (1998) 87
- Fifth-order two-dimensional vibrational spectroscopy of a Morse potential system in condensed phases, Y. Tanimura 233 (1998) 217
- Effects of non-Markovian relaxation in the femtosecond differential absorption spectra, E. Gaižauskas, A. Beržanskis and K.-H. Feller 235 (1998) 123
- Rotational relaxation of perylene in *n*-alcohols and *n*-alkanes studied by two-photon-induced anisotropy decay, S.W. Pauls, J.F. Hedstrom and C.K. Johnson 237 (1998) 205
- Investigation of spectral diffusion in PMMA on timescales from 10^{−5} to 10⁴ seconds via transient and photophysical hole burning, J. Müller, D. Haarer, O.V. Khodykin and B.M. Kharlamov 237 (1998) 483
- The second-harmonic response of single-crystal silver electrodes obtained with an interference method, G. Beltramo, C. Bilger, B. Pettinger and W. Schmickler 238 (1998) 473
- Nonlinear absorption and refraction in porphyrazine derivatives, C.Y. Tsai, S.P. Chen and T.C. Wen 240 (1999) 191
- Paramagnetic susceptibility simulations from crystal field effects on Nd³⁺ in magnesium borate MgNd(BO₂)₅, C. Cascales, R. Sáez Puche and P. Porcher 240 (1999) 291
- Synchrotron spectroscopies*
- A crossed molecular beam investigation of the reaction Cl + propane → HCl + C₃H₇ using VUV synchrotron radiation as a product probe, D.A. Blank, N. Hemmi, A.G. Suits and Y.T. Lee 231 (1998) 261
- On the electronic structure of Cu(III) and Ni(III) in La₂Li_{1/2}Cu_{1/2}O₄, Nd₂Li_{1/2}Ni_{1/2}O₄, and Cs₂KCuF₆, Z. Hu, G. Kaindl, S.A. Warda, D. Reinen, F.M.F. de Groot and B.G. Müller 232 (1998) 63

- Investigation of the CS_2^{2+} dication using threshold photoelectrons coincidence spectroscopy, M. Hochlaf, R.I. Hall, F. Penent, J.H.D. Eland and P. Lablanquie 234 (1998) 249
- Fragment ion yields from CFCl_3 photoexcited in regions of the $\text{Cl}2p$, the $\text{Cl}1s$, and the $\text{F}1s$ electron transitions, I.H. Suzuki and N. Saito 234 (1998) 255
- A study of the spectroscopic and thermodynamic properties of furan by means of photoabsorption, photoelectron and photoion spectroscopy, E.E. Rennie, C.A.F. Johnson, J.E. Parker, D.M.P. Holland, D.A. Shaw, M.A. MacDonald, M.A. Hayes and L.G. Shpinkova 236 (1998) 365
- The electronic structure of poly(pyridine-2,5-diyl) investigated by soft X-ray absorption and emission spectroscopies, M. Magnuson, L. Yang, J.-H. Guo, C. S  the, A. Agui, J. Nordgren, Y. Luo, H.   gren, N. Johansson, W.R. Salaneck, L.E. Horsburgh and A.P. Monkman 237 (1998) 295
- On the electronic spectroscopy of benzyl alcohol, J.M. Gingell, G. Marston, N.J. Mason, H. Zhao and M.R.F. Siggel 237 (1998) 443
- An experimental study of the valence shell photoelectron spectrum of the NO_2 molecule, P. Baltzer, L. Karlsson, B. Wannberg, D.M.P. Holland, M.A. MacDonald, M.A. Hayes and J.H.D. Eland 237 (1998) 451
- Threshold photoelectron spectroscopy of HCl and DCl , A.J. Yench, A.J. Cormack, R.J. Donovan, A. Hopkirk and G.C. King 238 (1998) 109
- Threshold photoelectron spectroscopy of HBr and DBr , A.J. Yench, A.J. Cormack, R.J. Donovan, K.P. Lawley, A. Hopkirk and G.C. King 238 (1998) 133
- Inner-shell excitation of PF_3 , PCl_3 , PCl_2CF_3 , OPF_3 and SPF_3 . Part I. Spectroscopy, J.J. Neville, A. J  rgensen, R.G. Cavell, N. Kosugi and A.P. Hitchcock 238 (1998) 201
- Reactivity of vinyl chloride ionic clusters, S. Martrenchard, C. Dedonder-Lardeux, I. Dimicoli, G. Gr  goire, C. Jouvet, M. Mons and D. Solgadi 239 (1998) 331
- Coherent optical spectroscopy*
- Vibrational coherence in bacterial reaction centers: spectroscopic characterisation of motions active during primary electron transfer, M.H. Vos, M.R. Jones and J.-L. Martin 233 (1998) 179
- Optical dephasing in photosynthetic pigment–protein complexes, H. Fidder, G.J.S. Fowler, C.N. Hunter and V. Sundstr  m 233 (1998) 311
- Atomic and molecular beam techniques*
- The correlation between the statistical properties of surface defect distribution and the specular intensity obtained from low energy He scattering technique, G. Petrella, L. Cassidei and F. Ciriaco 231 (1998) 31
- C–Br bond rupture in 193 nm photodissociation of vinyl bromide, H. Katayanagi, N. Yonekura and T. Suzuki 231 (1998) 345
- Charge transfer in gas–surface scattering: the three electronic state system, D. Guan, X. Yi, S. Ding, L. Gu and J.A. Olson 233 (1998) 35
- Ab initio calculations and supersonic jet studies on the geometry of 4-dimethylaminobenzonitrile (DMABN) and related compounds in the ground and excited state, U. Lommatzsch and B. Brutschy 234 (1998) 35
- Fragmentation pathways in the dissociation of fluoro-iodo-benzene negative ions, R.F.M. Lobo, A.M.C. Moutinho and M.J. Calhorda 234 (1998) 265
- On the electronic energy disposal of calcium excited atom reactions with halogen-containing compounds: Electronic branching ratio and spin–orbit state populations, M. Garay, C.A. Rinaldi, J.M. Orea and A. Gonz  lez Ure  a 236 (1998) 343

- Rotational alignment from the reactions $\text{Sr}(^3\text{P}_J) + \text{CCl}_4$ and CHCl_3 , M.-L. Wang, K.-L. Han, J.-P. Zhan, J.-H. Huang and G.-Z. He 236 (1998) 387
- Rotational spectra of the ^{15}N -aniline-X, (X = Ar, Ne) complexes. Structure determination from studies on isotopomers, V. Storm, H. Dreizler and D. Consalvo 237 (1998) 395
- An experimental test on the distribution of positronium lifetimes in polymers, G. Consolati, R. Rurali and M. Stefanetti 237 (1998) 493
- Rotational alignment from the $\text{Sr}(^3\text{P}_J) + \text{CH}_2\text{ClI}$ chemiluminescent reaction, M.-L. Wang, K.-L. Han, S.-L. Cong, G.-Z. He and N.-Q. Lou 238 (1998) 481
- Double resonance spectroscopy of phenol(H_2O) $_{1-12}$: evidence for ice-like structures in aromate–water clusters?, W. Roth, M. Schmitt, Ch. Jacoby, D. Spangenberg, Ch. Janzen and K. Kleinermanns 239 (1998) 1
- Investigations of OH–N- and NH–O-type hydrogen-bonded clusters by UV laser spectroscopy, C. Jacoby, P. Hering, M. Schmitt, W. Roth and K. Kleinermanns 239 (1998) 23
- Electronic spectroscopy and excited state dynamics of the Al–N $_2$ complex, X. Yang, I. Gerasimov and P.J. Dagdigan 239 (1998) 207
- Angular and velocity distributions of small cluster fragments in neutral (NH_3) $_n$ scattering off LiF(100), C. Menzel, R. Baumfalk and H. Zacharias 239 (1998) 287
- Capture dynamics in collisions between fullerene ions and rare gas atoms, E.E.B. Campbell, R. Ehlich, G. Heusler, O. Knospe and H. Sprang 239 (1998) 299
- Ultrafast dynamics of transition metal carbonyls. II. Picosecond evaporation after photodissociation of $\text{Cr}(\text{CO})_6 \cdot (\text{CH}_3\text{OH})_n$ heteroclusters at 280 nm, M. Gutmann, J.M. Janello and M.S. Dickebohm 239 (1998) 317
- Mode dependence of the state-to-state vibrational dynamics of HCN–HF, L. Oudejans and R.E. Miller 239 (1998) 345
- Vibrational and unimolecular dissociation of mixed solvent cluster ions: $\text{Na}^+((\text{CH}_3)_2\text{CO})_n(\text{CH}_3\text{OH})_m$, C.J. Weinheimer and J.M. Lisy 239 (1998) 357
- Stability and reactivity of hydrated magnesium cations, C. Berg, M. Beyer, U. Achatz, S. Joos, G. Niedner-Schatteburg and V.E. Bondybey 239 (1998) 379
- Photodissociation spectroscopy of (benzene–toluene) $^+$. Charge delocalization in the hetero-dimer ion, K. Ohashi, Y. Nakane, Y. Inokuchi, Y. Nakai and N. Nishi 239 (1998) 429
- Neutral and negatively-charged formamide, N-methylformamide and dimethylformamide clusters, C. Desfr  ois, V. P  riquet, S. Carles, J.P. Schermann and L. Adamowicz 239 (1998) 475
- Calculation of structures and vibrational spectra of acetonitrile clusters, J.G. Siebers, U. Buck and T.A. Beu 239 (1998) 549

Mass spectroscopy

- Direct observation of the equilibrium between cyclohexenyl radicals, O $_2$, and cyclohexenylperoxy radicals, R. Zils, S. Inomata, Y. Okunuki and N. Washida 231 (1998) 303
- Laser photodissociation of ketene at 230 nm, M. Castillejo, S. Couris, E. Lane, M. Martin and J. Ruiz 232 (1998) 353
- Fragment ion yields from CFCl_3 photoexcited in regions of the Cl2p, the Cl1s, and the F1s electron transitions, I.H. Suzuki and N. Saito 234 (1998) 255
- Dissociative photoionisation of NO $_2$ up to 26 eV, J.H.D. Eland and L. Karlsson 237 (1998) 139
- Reactions of solid glycine induced by keV ion irradiation, W. Huang, Z. Yu and Y. Zhang 237 (1998) 223
- Vertical double ionization of the sulphur dioxide molecule, I.W. Griffiths, D.E. Parry and F.M. Harris 238 (1998) 21
- Mass spectrometric and theoretical study of the mixed complex $\text{NaCeCl}_4(\text{g})$, J. Kapala, S. Roszak, I. Lisek and M. Miller 238 (1998) 221

- Penning ionization of C_{60} and C_{70} , J.M. Weber, K. Hansen, M.-W. Ruf and H. Hotop 239 (1998) 271
- Charge stripping effects from highly charged iodine ions formed from Coulomb explosion of CH_3I clusters, L. Poth, Q. Zhong, J.V. Ford, S.M. Hurley and A.W. Castleman Jr. 239 (1998) 309
- Photofragmentation dynamics of the $(N_2O)_2^+$ and $(N_2O)_3^+$ clusters: fragment N_2O^+ $A \leftarrow X$ spectra, S.A. Nizkorodov and E.J. Bieske 239 (1998) 369
- Stability and reactivity of hydrated magnesium cations, C. Berg, M. Beyer, U. Achatz, S. Joos, G. Niedner-Schatteburg and V.E. Bondybey 239 (1998) 379
- High-resolution electron ionization study of CO, $(CO)_2$ and $(CO)_3$: appearance energies and bond dissociation energies, D. Muigg, G. Denifl, A. Stamatovic, O. Echt and T.D. Märk 239 (1998) 409
- Photodissociation of $Mg^+-(CH_3OH)_N$ complexes: evidence for the onset of solvation, M.R. France, S.H. Pullins and M.A. Duncan 239 (1998) 447
- Threshold electron attachment and electron impact ionization involving oxygen dimers, J. Kreil, M.-W. Ruf, H. Hotop, I. Ettischer and U. Buck 239 (1998) 459

Radiolysis

- Positronium formation and quenching in frozen and liquid solutions in octanol, F. Bockstahl, I. Billard, G. Duplâtre and A. Bonnenfant 236 (1998) 393
- Reactions of solid glycine induced by keV ion irradiation, W. Huang, Z. Yu and Y. Zhang 237 (1998) 223

X-ray, electron and neutron diffraction

- An intermolecular potential function for Na^+ -acetonitrile obtained from ab initio calculations. Application to liquid simulations, E.M. Cabaleiro-Lago and M.A. Ríos 236 (1998) 235
- Paramagnetic susceptibility simulations from crystal field effects on Nd^{3+} in magnesium borate $MgNd(BO_2)_5$, C. Cascales, R. Sáez Puche and P. Porcher 240 (1999) 291

Neutron scattering (inelastic and quasielastic)

- The librational and vibrational spectra of water in natrolite, $Na_2Al_2Si_3O_{10} \cdot 2H_2O$ compared with ab-initio calculations, C.M.B. Line and G.J. Kearley 234 (1998) 207
- Rotational tunneling of methyl groups in the hydroquinone/acetonitrile clathrate: A combined deuteron NMR, INS, and computational study, A. Detken, P. Schiebel, M.R. Johnson, H. Zimmermann and U. Haeberlen 238 (1998) 301

Light scattering

- The electronic structure of poly(pyridine-2,5-diyl) investigated by soft X-ray absorption and emission spectroscopies, M. Magnuson, L. Yang, J.-H. Guo, C. Sâthe, A. Agui, J. Nordgren, Y. Luo, H. Ågren, N. Johansson, W.R. Salaneck, L.E. Horsburgh and A.P. Monkman 237 (1998) 295

Objects

Bulk systems

Gases

- Differential ring proton NMR shieldings and cyclic stabilization energies, D.B. Chesnut 231 (1998) 1
- High-resolution photoelectron spectroscopy using multibunch synchrotron radiation: rotational-resolved photoelectron bands of $O_2^+(b^4\Sigma_g^-, v^+)$, C.-W. Hsu, M. Evans, S. Stimson, C.Y. Ng and P. Heimann 231 (1998) 121

- Reactions of $N_2^+(v)$ with CO and NO at thermal energy, M.J. Frost, S. Kato, V.M. Bierbaum and S.R. Leone 231 (1998) 145
- Kinetic and mechanistic study of the reaction of atomic chlorine with methyl bromide over an extended temperature range, C.A. Piety, R. Soller, J.M. Nicovich, M.L. McKee and P.H. Wine 231 (1998) 155
- Photochemistry of acetone under tropospheric conditions, T. Gierczak, J.B. Burkholder, S. Bauerle and A.R. Ravishankara 231 (1998) 229
- New results on the atmospheric photooxidation of simple alkylbenzenes, B. Klotz, I. Barnes and K.H. Becker 231 (1998) 289
- Direct observation of the equilibrium between cyclohexenyl radicals, O_2 , and cyclohexenylperoxy radicals, R. Zils, S. Inomata, Y. Okunuki and N. Washida 231 (1998) 303
- Spin-orbit branching in the predissociation of the $C^1\Pi$ state of HCl and DCl: a manifestation of quantum interference, M.H. Alexander, X. Li, R. Liyanage and R.J. Gordon 231 (1998) 331
- Hartree-Fock limit properties of the water dimer in absence of BSSE, A. Famulari, M. Raimondi, M. Sironi and E. Gianinetti 232 (1998) 275
- Ab initio MO-VB study of water dimer, A. Famulari, M. Raimondi, M. Sironi and E. Gianinetti 232 (1998) 289
- A density functional study of weakly bound hydrogen bonded complexes, A.K. Chandra and M.T. Nguyen 232 (1998) 299
- Towards quantitative diatomics-in-molecules model for the water molecule, B.L. Grigorenko, A.V. Nemukhin and V.A. Apkarian 232 (1998) 321
- Classical and quantum dynamics on the collinear potential energy surface for the reaction of Li with H_2 , N.J. Clarke, M. Sironi, M. Raimondi, S. Kumar, F.A. Gianturco, E. Buonomo and D.L. Cooper 233 (1998) 9
- Transport properties of a reacting gas mixture with strong vibrational and chemical nonequilibrium, E.V. Kustova and E.A. Nagnibeda 233 (1998) 57
- Free energies of solvation for peptides and polypeptides using SCRF methods, C. Alemán, H.M. Ishiki, E.A. Armelin, O. Abrahão Junior and S.E. Galembeck 233 (1998) 85
- Populations of rotational levels of nitrogen molecules in free jets. Comparison of CARS and electron beam fluorescent technique, R.G. Sharafutdinov, A.A. Ilyukhin, V.V. Smirnov, A.E. Belikov, G.I. Sukhinin and R.L. Pykhov 233 (1998) 127
- A He(I) photoelectron spectroscopic study of the \tilde{X}^2A_2 state of NH_3^+ and ND_3^+ . A reanalysis and evidence for the coriolis coupling between the bending ν_2 and ν_4 modes, R. Loch, B. Leyh, K. Hottmann and H. Baumgärtel 233 (1998) 145
- An ab initio study of NMR isotropic shielding bond length derivatives in phosphorus compounds, A. Dransfeld and D.B. Chesnut 234 (1998) 69
- Infrared spectra of polycyclic aromatic hydrocarbons: methyl substitution and loss of H, C.W. Bauschlicher, Jr. and S.R. Langhoff 234 (1998) 79
- Solvent effects on NMR spectrum of acetylene calculated by ab initio methods, M. Pecul and J. Sadlej 234 (1998) 111
- REMPI spectroscopy of internal state populations in $HBr + Ar$ free jets: Rotational relaxation of HBr, A.E. Belikov, M.M. Ahern and M.A. Smith 234 (1998) 195
- Binary collision theory for thermal and nonisothermal relaxation and reaction of polyatomic molecules, P. Talkner, E. Pollak and A.M. Berezhkovskii 235 (1998) 131
- CARS studies of bending states of CO_2 : evidence of collisional rotational transitions with odd ΔJ , A.P. Kouzov, D.N. Kozlov and B. Hemmerling 236 (1998) 15

- Ultraviolet absorption spectrum and cross-sections of vinyl (C_2H_3) radical in the 225–238 nm region, A. Fahr, P. Hassanzadeh and D.B. Atkinson 236 (1998) 43
- On the $O_2(v') + O_2(v'')$ atmospheric reaction. II. The role of rotational excitation, W. Wang and A.J.C. Varandas 236 (1998) 181
- Emission spectra of $HeAr_2^+$ and $HeKr_2^+$ heterotrimer ions produced in a helium flowing afterglow, M. Tsuji, M. Tanaka, E. Oda, H. Ishimi and Y. Nishimura 236 (1998) 319
- The mechanism of the $CH_3O + CO$ reaction and the stability of the CH_3OCO radical, J.S. Francisco 237 (1998) 1
- Linear response calculations of electronic g -factors and spin-rotational coupling constants for diatomic molecules with a triplet ground state, M. Engström, B. Minaev, O. Vahtras and H. Ågren 237 (1998) 149
- Reactions of $C(^1D)$ with H_2 , HD and D_2 : kinetic isotope effect and the CD/CH branching ratio, K. Sato, N. Ishida, T. Kurakata, A. Iwasaki and S. Tsunashima 237 (1998) 195
- Interaction anisotropy and quantum dynamics for vibrationally inelastic collisions of $LiH(^1\Sigma)$ with $He(^1S)$, E. Bodo, E. Buonomo, F.A. Gianturco, S. Kumar, A. Famulari, M. Raimondi and M. Sironi 237 (1998) 315
- On the electronic spectroscopy of benzyl alcohol, J.M. Gingell, G. Marston, N.J. Mason, H. Zhao and M.R.F. Siggel 237 (1998) 443
- Complete basis set limit ionization potentials of O_3 and NO_2 using the multiconfigurational spin tensor electron propagator method (MCSTEP), A.J. McKellar, D. Heryadi, D.L. Yeager and J.A. Nichols 238 (1998) 1
- Analysis of the reaction paths to dissociation of dichloro-ethylenes into Cl_2 and C_2H_2 , S.M. Resende and W.B. De Almeida 238 (1998) 11
- Ab initio study of the electronic spectrum of $C_2H_2^+$. I. Vertical spectrum and angular potential curves, M. Perić, B. Engels and M. Hanrath 238 (1998) 33
- Ab initio study of the electronic spectrum of $C_2H_2^+$. II. Stretching potential energy surfaces for low-lying doublet electronic states, M. Perić and B. Engels 238 (1998) 47
- Threshold photoelectron spectroscopy of HCl and DCl, A.J. Yench, A.J. Cormack, R.J. Donovan, A. Hopkirk and G.C. King 238 (1998) 109
- Threshold photoelectron spectroscopy of HBr and DBr, A.J. Yench, A.J. Cormack, R.J. Donovan, K.P. Lawley, A. Hopkirk and G.C. King 238 (1998) 133
- The electronic states of pyrrole studied by optical (VUV) absorption, near-threshold electron energy-loss (EEL) spectroscopy and ab initio multi-reference configuration interaction calculations, M.H. Palmer, I.C. Walker and M.F. Guest 238 (1998) 179
- Inner-shell excitation of PF_3 , PCl_3 , PCl_2CF_3 , OPF_3 and SPF_3 . Part I. Spectroscopy, J.J. Neville, A. Jürgensen, R.G. Cavell, N. Kosugi and A.P. Hitchcock 238 (1998) 201
- New investigation of the photodissociation of the HBr molecule: total cross-section, anisotropy parameter and dependence of the spin-orbit branching on the ground state vibrational level, B. Pouilly and M. Monnerville 238 (1998) 437
- Rotational alignment from the $Sr(^3P_J) + CH_2ClI$ chemiluminescent reaction, M.-L. Wang, K.-L. Han, S.-L. Cong, G.-Z. He and N.-Q. Lou 238 (1998) 481
- Highly resolved UV spectroscopy of clusters: isotope substitution studies of hydrogen-bonded phenol · water, R.M. Helm and H.J. Neusser 239 (1998) 33
- On the nonequilibrium effects in thermally activated reactions $A + A \rightleftharpoons B + B \rightleftharpoons C + C$, J. Gorecki and J.N. Gorecka 240 (1999) 215
- A Keilson–Storer type collision kernel for rotation–translation coupling, M.F. Gelin 240 (1999) 265
- Vibrational excitation of the $C^3\Pi_u$ state of N_2 by electron impact, G. Poparić, M. Vičić and D.S. Belić 240 (1999) 283

Supersonic beams

- C–Br bond rupture in 193 nm photodissociation of vinyl bromide, H. Katayanagi, N. Yonekura and T. Suzuki 231 (1998) 345
- Fluorescence lifetime of rovibrational states of h_4 -acetaldehyde and spectra of d_4 -acetaldehyde, S.-H. Jen, T.-J. Hsu and I.-C. Chen 232 (1998) 131
- Laser photodissociation of ketene at 230 nm, M. Castillejo, S. Couris, E. Lane, M. Martin and J. Ruiz 232 (1998) 353
- Model study of proton transfer in a H-bonded cluster with an A–H...B reaction complex. Introduction of an effective coordinate for the solvation shell, M.V. Vener 233 (1998) 77
- Ab initio calculations and supersonic jet studies on the geometry of 4-dimethylamino-benzonitrile (DMABN) and related compounds in the ground and excited state, U. Lommatzsch and B. Brutschy 234 (1998) 35
- Rotational spectra of the ^{15}N -aniline–X, (X = Ar, Ne) complexes. Structure determination from studies on isotopomers, V. Storm, H. Dreizler and D. Consalvo 237 (1998) 395
- ‘Anomalous’ density of states and rotational selection rules of loosely bound states of NO_2 , A. Delon, S. Heilliette and R. Jost 238 (1998) 465
- Electronic spectroscopy of jet-cooled anthracene/ $(\text{H}_2\text{O})_n$ clusters ($n = 1–16$): comparisons of inhomogeneous structure, P.M. Palmer and M.R. Topp 239 (1998) 65
- Existence of two internal energy distributions in jet-formed van der Waals heteroclusters: example of the anthracene–argon $_n$ system, D. Uridat, V. Brenner, I. Dimicoli, J. Le Calvé, P. Millié, M. Mons and F. Piuze 239 (1998) 151
- Electronic spectroscopy and excited state dynamics of the Al– N_2 complex, X. Yang, I. Gerasimov and P.J. Dagdigan 239 (1998) 207
- Large-amplitude motion in highly quantum clusters: high-resolution infrared absorption studies of jet-cooled H_2 –HCl and H_2 –DCI, D.T. Anderson, M. Schuder and D.J. Nesbitt 239 (1998) 253
- Angular and velocity distributions of small cluster fragments in neutral $(\text{NH}_3)_n$ scattering off LiF(100), C. Menzel, R. Baumfalk and H. Zacharias 239 (1998) 287
- Charge stripping effects from highly charged iodine ions formed from Coulomb explosion of CH_3I clusters, L. Poth, Q. Zhong, J.V. Ford, S.M. Hurley and A.W. Castleman Jr. 239 (1998) 309
- High-resolution electron ionization study of CO, $(\text{CO})_2$ and $(\text{CO})_3$: appearance energies and bond dissociation energies, D. Muigg, G. Denifl, A. Stamatovic, O. Echt and T.D. Märk 239 (1998) 409
- Photodissociation spectroscopy of (benzene–toluene) $^+$. Charge delocalization in the hetero-dimer ion, K. Ohashi, Y. Nakane, Y. Inokuchi, Y. Nakai and N. Nishi 239 (1998) 429
- Photodissociation of $\text{Mg}^+-(\text{CH}_3\text{OH})_N$ complexes: evidence for the onset of solvation, M.R. France, S.H. Pullins and M.A. Duncan 239 (1998) 447
- Competition between electronic and vibrational predissociation in Ar– $\text{I}_2(B)$: a molecular dynamics with quantum transitions study, A. Bastida, J. Zuñiga, A. Requena, N. Halberstadt and J.A. Beswick 240 (1999) 229

Liquids neat

- Water anomalies and the double-well Takahashi model, C.H. Cho, S. Singh and G.W. Robinson 232 (1998) 329
- Quantum time correlation functions and classical coherence, R. Hernandez and G.A. Voth 233 (1998) 243
- A viscoelastic continuum model of non-polar solvation. II. Vibrational dephasing in moderate to high-viscosity liquids and glasses, M.A. Berg and H.W. Hubble 233 (1998) 257
- Population relaxation and non-Markovian frequency fluctuations in third- and fifth-order Raman scattering, T. Steffen and K. Duppen 233 (1998) 267

- Vibrational energy relaxation in liquid oxygen, K.F. Everitt, S.A. Egorov and J.L. Skinner 235 (1998) 115
- An ab initio time-dependent Hartree–Fock study of solvent effects on the polarizability and second hyperpolarizability of polyacetylene chains within the polarizable continuum model, B. Champagne, B. Mennucci, M. Cossi, R. Cammi and J. Tomasi 238 (1998) 153
- Ab initio theoretical optical rotations of small molecules, P.L. Polavarapu and D.K. Chakraborty 240 (1999) 1
- On the nonequilibrium effects in thermally activated reactions $A + A \rightleftharpoons B + B \rightleftharpoons C + C$, J. Gorecki and J.N. Gorecka 240 (1999) 215
- Liquid mixtures and solutions*
- ¹³C NMR relaxation in neutral and charged tetra-*n*-alkyl compounds, B. Bordes, F. Coletta, A. Ferrarini, F. Gottardi and P.L. Nordio 231 (1998) 51
- A frequency-resolved cavity model (FRCM) for treating equilibrium and non-equilibrium solvation energies, M.V. Basilevsky, I.V. Rostov and M.D. Newton 232 (1998) 189
- A frequency-resolved cavity model (FRCM) for treating equilibrium and non-equilibrium solvation energies. 2: Evaluation of solvent reorganization energies, M.D. Newton, M.V. Basilevsky and I.V. Rostov 232 (1998) 201
- Vibrational energy transfer processes in dye molecules after ultrafast excitation of skeletal modes, T. Dahinten, J. Baier and A. Seilmeier 232 (1998) 239
- Molecular dynamics studies of NaCl solutions in methanol–water mixtures. An effect of NaCl on hydrogen bonded network, E. Hawlicka and D. Swiatla-Wojcik 232 (1998) 361
- Free energies of solvation for peptides and polypeptides using SCRF methods, C. Alemán, H.M. Ishiki, E.A. Armelin, O. Abrahão Junior and S.E. Galembeck 233 (1998) 85
- Controlling condensed-phase vibrational excitation with tailored infrared pulses, V.D. Kleiman, S.M. Arrivo, J.S. Melinger and E.J. Heilweil 233 (1998) 207
- Heterodyne-detected stimulated photon echo: applications to optical dynamics in solution, W.P. de Boeij, M.S. Pshenichnikov and D.A. Wiersma 233 (1998) 287
- The steady-state Green's function theory in monomolecular reactions. II. Effects of solvent dynamics and non-equilibrium initial distributions in reactions on position-dependent transition regions, O.B. Jenkins and A.B. Doktorov 234 (1998) 121
- Curvilinear-path based theory of the energy transfer limited rate of a two-dimensional solute in a dissipative bath, S.K. Reese and S.C. Tucker 235 (1998) 171
- Reversible chemical reactions in slowly relaxing environments: Kramers' turnover of the rate constant, A.M. Berezhkovskii, V.Yu. Zitserman, D.-Y. Yang and S.H. Lin 235 (1998) 201
- Phase space distribution function approach to the Kramers problem. III. Anharmonic potentials, J. Morelli and D.J. Tannor 235 (1998) 213
- Photochemical accumulation and recombination of ion pairs undergoing the singlet–triplet conversion, A.I. Burshtein and A.Yu. Sivachenko 235 (1998) 257
- Non-adiabatic effects in condensed phase activated rate processes in the near-adiabatic limit, A.I. Shushin and M. Tachiya 235 (1998) 267
- Non-equilibrium interlevel transitions in condensed phase far away from the avoided crossing region, M.V. Basilevsky, A.V. Soudackov and A.I. Voronin 235 (1998) 281
- Numerical simulations of solvation in simple polar fluids: dependence on the thermodynamic state below and above the critical point, P. Graf and A. Nitzan 235 (1998) 297
- Femtosecond pump–probe studies of chlorine dioxide photochemistry in water and acetonitrile, M.J. Philpott, S.C. Hayes and P.J. Reid 236 (1998) 207
- An intermolecular potential function for Na⁺–acetonitrile obtained from ab initio calculations. Application to liquid simulations, E.M. Cabaleiro-Lago and M.A. Ríos 236 (1998) 235

- Vibrational spectroscopy and molecular dynamics of solvated methanol tetramer and pentamer, D. Meyer zum Büschenfelde and A. Staib 236 (1998) 253
- Analytical theory of time-resolved fluorescence anisotropy and dynamic stokes shift of polar solute molecules based on continuum model for solvent, F. Tanaka and N. Mataga 236 (1998) 277
- Photophysical and lasing properties of pyrromethene 567 dye in liquid solution. Environment effects, F. López Arbeloa, T. López Arbeloa, I. López Arbeloa, I. García-Moreno, A. Costela, R. Sastre and F. Amat-Guerri 236 (1998) 331
- Positronium formation and quenching in frozen and liquid solutions in octanol, F. Bockstahl, I. Billard, G. Duplâtre and A. Bonnenfant 236 (1998) 393
- Modelling the substitution effects of several rhodium(III) transition metal complexes using the angular overlap model, B. Gilliams, D. Vandenbroucke and C. Görller-Walrand 237 (1998) 91
- Rotational relaxation of perylene in *n*-alcohols and *n*-alkanes studied by two-photon-induced anisotropy decay, S.W. Pauls, J.F. Hedstrom and C.K. Johnson 237 (1998) 205
- Peculiarity of triplet–triplet energy transfer from 2-(2'-hydroxy-phenyl)benzoxazole to diacetyl. Evidence for radiative keto–enol transitions $^3K^* \rightarrow ^1E$ and $^1E \rightarrow ^1K^*$, B. Nickel and P.J. Walla 237 (1998) 371
- IR–IR double-resonance studies of vibrational relaxation of CD₃F in solid and liquid Xe, Kr, Ar solutions near the melting point, K.S. Rutkowski 237 (1998) 403
- On the dielectric continuum solvent model for theoretical estimates of the conformational equilibrium of molecules with an intramolecular hydrogen bond, T. Yasuda and S.-i. Ikawa 238 (1998) 173
- Wavelength dependence of the nonlinear absorption properties of laser dyes in solid and liquid solutions, J. Barroso, A. Costela, I. García-Moreno and R. Sastre 238 (1998) 257
- Manifestation of interaction of the transition dipole moments in IR spectra of low-temperature liquids and solutions in liquefied noble gases, T.D. Kolomiitsova, A.P. Burtsev, V.G. Fedoseev and D.N. Shchepkin 238 (1998) 315
- Solvent effects within the CS INDO method. Geometrical distortion and solvatochromism of merocyanine dyes, I. Baraldi, F. Momicchioli, G. Ponterini and D. Vanossi 238 (1998) 353
- Experimental and theoretical studies of the low-lying electronic states of the simplest benzylic amide [2]catenane, A.M. Brouwer, W.J. Buma, R. Caudano, M. Fanti, C.-A. Fustin, D.A. Leigh, A. Murphy, P. Rudolf, F. Zerbetto and J.M. Zwier 238 (1998) 421
- Raman spectroscopy study on the dynamic behavior of nitrate anion in zinc nitrate solution at high temperatures and pressure, Y. Ikushima and M. Arai 238 (1998) 455
- Laser driven hydrogen tunneling in a dissipative environment, H. Naundorf, K. Sundermann and O. Kühn 240 (1999) 163
- Cavitation contribution to the free energy of solvation. Comparison of different formalisms in the context of MST calculations, C. Colominas, F.J. Luque, J. Teixidó and M. Orozco 240 (1999) 253
- A Keilson–Storer type collision kernel for rotation–translation coupling, M.F. Gelin 240 (1999) 265
- Electric field effect on the upper critical solution temperature, K. Orzechowski 240 (1999) 275
- Are the changes in the lifetime of the excited uranyl ion of chemical or physical nature?, M. Bouby, I. Billard, A. Bonnenfant and G. Klein 240 (1999) 353

Crystals

- Effect of pressure and temperature on the H-atom tunneling in solid phase chemical reactions. The acridine/fluorene system, L.I. Trakhtenberg and V.L. Klochikhin 232 (1998) 175
- The librational and vibrational spectra of water in natrolite, Na₂Al₂Si₃O₁₀ · 2H₂O compared with ab-initio calculations, C.M.B. Line and G.J. Kearley 234 (1998) 207
- Field-induced localization and nonlinear response of a one-band conductor to a periodic electric field, A.A. Ovchinnikov and K.A. Pronin 235 (1998) 93

- A comparative study of the electronic structure of α -MnS (alabandite) calculated at the Hartree-Fock and Density Functional levels of theory, R. Tappero and A. Lichanot 236 (1998) 97
- Electronic structure of planar superconducting systems. From finite to extended model, S. Larsson 236 (1998) 133
- Role of the local electric field in electro-absorption spectra of molecular crystals, R.W. Munn 236 (1998) 151
- Classical energy calculations with electron correlation of condensed excited states — Rydberg Matter, L. Holmlid 237 (1998) 11
- Electron paramagnetic resonance of Er^{3+} doped in YVO_4 : hyperfine parameters, S.K. Misra, S. Isber, J.A. Capobianco and E. Cavalli 240 (1999) 313
- Comparative study of the spectroscopic properties of Cr^{4+} -doped LiAlO_2 and LiGaO_2 , S. Kück and S. Hartung 240 (1999) 387
- neat*
- ^{17}O quadrupole coupling in $\text{C}-\text{O}-\text{H} \cdots \text{O}=\text{C}$ hydrogen bonds, J. Seliger 231 (1998) 81
- ^{17}O nuclear quadrupole resonance study of proton disorder in solid benzoic acid, 4-hydroxybenzoic acid and 4-nitrobenzoic acid, J. Seliger and V. Žagar 234 (1998) 223
- Field-induced localization and nonlinear response of a one-band conductor to a periodic electric field, A.A. Ovchinnikov and K.A. Pronin 235 (1998) 93
- Theoretical study of the crystal field excitations in CoO , C. de Graaf, W.A. de Jong, R. Broer and W.C. Nieuwpoort 237 (1998) 59
- Rotational tunneling of methyl groups in the hydroquinone/acetonitrile clathrate: A combined deuteron NMR, INS, and computational study, A. Detken, P. Schiebel, M.R. Johnson, H. Zimmermann and U. Haeberlen 238 (1998) 301
- mixed*
- Perylene in biphenyl and anthracene crystals: an example of the influence of the host on single-molecule signals, P.J. Walla, F. Jelezko, Ph. Tamarat, B. Lounis and M. Orrit 233 (1998) 117
- Wavepacket diagnosis with chirped probe pulses, R. Zadoyan, N. Schwentner and V.A. Apkarian 233 (1998) 353
- Model calculations of local exciton levels in the C_{60} fullerene crystals doped with endohedral fullerenes $\text{M}@\text{C}_{60}$, A. Eilmes and P. Petelenz 237 (1998) 67
- IR–IR double-resonance studies of vibrational relaxation of CD_3F in solid and liquid Xe, Kr, Ar solutions near the melting point, K.S. Rutkowski 237 (1998) 403
- Glasses*
- Hole trapping in tri-*p*-tolylamine-doped poly(styrene), P.M. Borsenberger, W.T. Gruenbaum, U. Wolf and H. Bässler 234 (1998) 277
- Isotope effect in diffusion of methyl radicals in glassy ethanol-1,2- d_5 at low temperatures, V.L. Vyazovkin and V.A. Tolkatchev 236 (1998) 291
- Transport kinetics of triplet excitation in solid chrysene, S.A. Bagnich 237 (1998) 359
- Investigation of spectral diffusion in PMMA on timescales from 10^{-5} to 10^4 seconds via transient and photophysical hole burning, J. Müller, D. Haarer, O.V. Khodykin and B.M. Kharlamov 237 (1998) 483
- Complex fluids*
- On the dependence of a critical supersaturation on pressure of a two-component background gas in a diffusion cloud chamber, A.L. Itkin 238 (1998) 273

- Solvent effects on outersphere electron transfer reactions in mixed dipolar liquids, A. Chandra 238 (1998) 285
- liquid crystals*
- A diffusive model for interpreting solvation dynamics in isotropic and ordered liquid phases, A. Polimeno, G. Saielli and P.L. Nordio 235 (1998) 313
- colloidal suspensions*
- Electrical properties of a charged surface in a general electrolyte solution, Y.-C. Kuo and J.-P. Hsu 236 (1998) 1
- Electrical interaction between two spherical particles covered by an ion-penetrable charged membrane, J.-P. Hsu and B.-T. Liu 236 (1998) 63
- Polymers*
- Optical limiting properties of a zinc porphyrin polymer and its dimer and monomer model compounds, F.M. Qureshi, S.J. Martin, X. Long, D.D.C. Bradley, F.Z. Henari, W.J. Blau, E.C. Smith, C.H. Wang, A.K. Kar and H.L. Anderson 231 (1998) 87
- Hole trapping in tri-*p*-tolylamine-doped poly(styrene), P.M. Borsenberger, W.T. Gruenbaum, U. Wolf and H. Bässler 234 (1998) 277
- Photogeneration of charge in solid films of α -sexithiophene, J. Kalinowski, W. Stampor, P. Di Marco and F. Garnier 237 (1998) 233
- Correlation corrected energy bands of nucleotide base stacks, F. Bogár and J. Ladik 237 (1998) 273
- Dielectric effects of step-increased pressure on the mass- and diffusion-controlled linear chain and network macromolecules growth, D.A. Wasylyshyn and G.P. Johari 237 (1998) 345
- An experimental test on the distribution of positronium lifetimes in polymers, G. Consolati, R. Rurali and M. Stefanetti 237 (1998) 493
- Volume phase transition of polymer gel in water and heavy water, H. Shirota, N. Endo and K. Horie 238 (1998) 487
- Hole transport in arylamine doped polymers, S.A. Visser, W.T. Gruenbaum, E.H. Magin and P.M. Borsenberger 240 (1999) 197
- Semiconductors*
- High frequency satellites in resonant activation, E. Turlot, S. Linkwitz, D. Esteve, C. Urbina, M.H. Devoret and H. Grabert 235 (1998) 47
- Metals and alloys*
- A theoretical study of the electronic structure and spectroscopic properties of the low-lying electronic states of the molecule AlSi, F.R. Ornellas and S. Iwata 232 (1998) 95
- Thin films*
- Optical limiting properties of a zinc porphyrin polymer and its dimer and monomer model compounds, F.M. Qureshi, S.J. Martin, X. Long, D.D.C. Bradley, F.Z. Henari, W.J. Blau, E.C. Smith, C.H. Wang, A.K. Kar and H.L. Anderson 231 (1998) 87
- Quantum superconductor-metal transition in a 2D proximity-coupled array, M.V. Feigel'man and A.I. Larkin 235 (1998) 107
- Photogeneration of charge in solid films of α -sexithiophene, J. Kalinowski, W. Stampor, P. Di Marco and F. Garnier 237 (1998) 233

Surfaces

- The correlation between the statistical properties of surface defect distribution and the specular intensity obtained from low energy He scattering technique, G. Petrella, L. Cassidei and F. Ciriaco 231 (1998) 31
- Molecular relaxation in simple dipolar liquids confined between two solid surfaces, S. Senapati and A. Chandra 231 (1998) 65
- Dependence of volume-produced H^- ions on the wall recombination probability of H atoms in a low pressure H_2 positive column, J. Loureiro and J. Amorim 232 (1998) 141
- Charge transfer in gas–surface scattering: the three electronic state system, D. Guan, X. Yi, S. Ding, L. Gu and J.A. Olson 233 (1998) 35
- Interference-effects in the laser-induced desorption of small molecules from surfaces: a model study, S. Thiel, T. Klüner and H.-J. Freund 236 (1998) 263
- The energy relaxation of Si–H vibration in the H/Si(111) system. Relaxation rate and potential energy surface anharmonicity, V.A. Ermoshin, A.K. Kazansky, K.S. Smirnov and D. Bougeard 237 (1998) 333
- Quantum study of oriented NO scattering from Ag(111): orientational steering and effects of surface corrugation, D. Lemoine and T. Duhoo 238 (1998) 59
- Experimental and theoretical studies of the low-lying electronic states of the simplest benzylic amide [2]catenane, A.M. Brouwer, W.J. Buma, R. Caudano, M. Fanti, C.-A. Fustin, D.A. Leigh, A. Murphy, P. Rudolf, F. Zerbetto and J.M. Zwier 238 (1998) 421
- Angular and velocity distributions of small cluster fragments in neutral $(NH_3)_n$ scattering off LiF(100), C. Menzel, R. Baumfalk and H. Zacharias 239 (1998) 287

Low-dimensional materials

- A Valence-Bond/Hartree–Fock method to determine the Hubbard transfer integrals in organic conductors, F. Castet, L. Ducasse and A. Fritsch 232 (1998) 37
- Vibrational modes in layered double hydroxides and their calcined derivatives, W. Kagnya, R. Baddour-Hadjean, F. Kooli and W. Jones 236 (1998) 225
- Transport kinetics of triplet excitation in solid chrysene, S.A. Bagnich 237 (1998) 359
- Quantum motion of particles along one-dimensional pathways with static and dynamic energy disorder, L.D.A. Siebbeles and Y.A. Berlin 238 (1998) 97
- Nonlinear absorption and refraction in porphyrazine derivatives, C.Y. Tsai, S.P. Chen and T.C. Wen 240 (1999) 191

Dielectrics

- Molecular relaxation in simple dipolar liquids confined between two solid surfaces, S. Senapati and A. Chandra 231 (1998) 65
- A diffusive model for interpreting solvation dynamics in isotropic and ordered liquid phases, A. Polimeno, G. Saielli and P.L. Nordio 235 (1998) 313
- Cold photoconductivity in a system of interacting charge-transfer excitons at a donor–acceptor interface, S.A. Kiselev, E. Hartung, Z.G. Soos, S.R. Forrest and V.M. Agranovich 238 (1998) 365

Plasmas

- Generalization of the Arrhenius relation and ionization reaction rates for carbon atoms and ions in plasmas, Y. Chang and C.A. Ordonez 231 (1998) 27
- Dependence of volume-produced H^- ions on the wall recombination probability of H atoms in a low pressure H_2 positive column, J. Loureiro and J. Amorim 232 (1998) 141

- Nonequilibrium dissociation of hydrogen in a parallel-plate radio frequency discharge, S. Longo and I.D. Boyd 238 (1998) 445

Biological systems

- Mathematical aspects of the fluctuating barrier problem. Existence of equilibrium and relaxation solutions, P. Pechukas and J. Ankerhold 235 (1998) 5
- Recognition and characterization of binding modes of Δ - and Λ -[Ru(phen)₃]²⁺ and Δ - and Λ -[Ru(phen)₂DPPZ]²⁺ by the ²³Na NMR relaxation and binding free energy parameters, F.C. Marincola, M. Casu, G. Saba, A. Lai, P. Lincoln and B. Nordén 236 (1998) 301
- Sub-picosecond excited-state dynamics of a carotenoid (spirilloxanthin) in the light-harvesting systems of *Chromatium vinosum*. Relaxation process from the optically allowed S₂ state, H. Okamoto, M. Ogura, T. Nakabayashi and M. Tasumi 236 (1998) 309
- Correlation corrected energy bands of nucleotide base stacks, F. Bogár and J. Ladik 237 (1998) 273
- Impedance spectroscopic investigation of the temperature influence on the transfer of tetraphenylborate ions through lipid membranes — Calculation of energy barriers for the ion transfer across lipid membranes, K.-D. Schulze 238 (1998) 495
- L-Alanyl-L-alanine in the zwitterionic state: structures determined in the presence of explicit water molecules and with continuum models using density functional theory, M. Knapp-Mohammady, K.J. Jalkanen, F. Nardi, R.C. Wade and S. Suhai 240 (1999) 63

Microscopic and mesoscopic systems

Single atoms, molecules and assemblies (incl. biological)

- Theoretical study of the Cl 1s and 2p near edge photoabsorption spectra of HCl by accurate ab-initio configuration interaction and density functional approaches, G. Fronzoni, M. Stener, P. Decleva and G. De Alti 232 (1998) 9
- Accurate universal basis set for H through Xe for Hartree–Fock calculations, F.E. Jorge and R.F. Martins 233 (1998) 1
- Classical and quantum dynamics on the collinear potential energy surface for the reaction of Li with H₂, N.J. Clarke, M. Sironi, M. Raimondi, S. Kumar, F.A. Gianturco, E. Buonomo and D.L. Cooper 233 (1998) 9
- Perylene in biphenyl and anthracene crystals: an example of the influence of the host on single-molecule signals, P.J. Walla, F. Jelezko, Ph. Tamarat, B. Lounis and M. Orrit 233 (1998) 117
- Suppression of quantum coherence: Noise effect, J. Shao, C. Zerbe and P. Hänggi 235 (1998) 81
- The Kramers problem in 2D-coupled periodic potentials, G. Caratti, R. Ferrando, R. Spadacini and G.E. Tommei 235 (1998) 157
- Study of positronium hydride with a simple wavefunction: Application to the Stark effect of PsH, C. Le Sech and B. Silvi 236 (1998) 77
- On the accuracy of averaged relativistic shape-consistent pseudopotentials, L. Maron and C. Teichteil 237 (1998) 105
- A rigorous quantum molecular dynamics study of a collinear A + BC → AB + C reaction, L. Wang 237 (1998) 305
- Semiclassical reactive scattering: the Hermite correction method in hyperspherical coordinates, S. Adhikari and G.D. Billing 238 (1998) 69
- Rotational alignment from the Sr(³P_J) + CH₂ClI chemiluminescent reaction, M.-L. Wang, K.-L. Han, S.-L. Cong, G.-Z. He and N.-Q. Lou 238 (1998) 481
- Radical-substituted allenes as high-spin species and subunits of organic ferromagnets, R. Beust, N. Tyutyulkov, M. Rabinovitz and F. Dietz 240 (1999) 141

- A gas phase ab initio excited state geometry optimization study of thymine, cytosine and uracil, M.K. Shukla and P.C. Mishra 240 (1999) 319
- Molecules (neutral and ionic)*
- Theoretical study of the OH + NO₂ reaction: formation of nitric acid and the hydroperoxyl radical, D. Chakraborty, J. Park and M.C. Lin 231 (1998) 39
- ¹³C NMR relaxation in neutral and charged tetra-*n*-alkyl compounds, B. Bordes, F. Coletta, A. Ferrarini, F. Gottardi and P.L. Nordio 231 (1998) 51
- Spin-forbidden dissociation of ozone in the Huggins bands, W. Denzer, G. Hancock, J.C. Pinot de Moira and P.L. Tyley 231 (1998) 109
- Translational energy and angular distributions of O(¹D) and O(³P_j) fragments in the UV photodissociation of ozone, K. Takahashi, N. Taniguchi, Y. Matsumi and M. Kawasaki 231 (1998) 171
- Monte Carlo calculation of partition functions for straight chain alkanes, J. Gang, M.J. Pilling and S.H. Robertson 231 (1998) 183
- On the UV photodissociation dynamics of hydrogen iodide, S.R. Langford, P.M. Regan, A.J. Orr-Ewing and M.N.R. Ashfold 231 (1998) 245
- A crossed molecular beam investigation of the reaction Cl + propane → HCl + C₃H₇ using VUV synchrotron radiation as a product probe, D.A. Blank, N. Hemmi, A.G. Suits and Y.T. Lee 231 (1998) 261
- Infrared spectra of polycyclic aromatic hydrocarbons: oxygen substitution, C.W. Bauschlicher, Jr. 233 (1998) 29
- Free energies of solvation for peptides and polypeptides using SCRF methods, C. Alemán, H.M. Ishiki, E.A. Armelin, O. Abrahão Junior and S.E. Galembeck 233 (1998) 85
- Femtosecond photodissociation of triiodide in solution: Excitation energy dependence and transition state dynamics, T. Kühne, R. Küster and P. Vöhringer 233 (1998) 161
- The intermolecular interaction mechanisms in liquid CS₂ at 295 and 165 K probed with two-dimensional Raman spectroscopy, A. Tokmakoff, M.J. Lang, X.J. Jordanides and G.R. Fleming 233 (1998) 231
- Intramolecular proton transfer in the ground and the two lowest-lying singlet excited states of 1-amino-3-propenal and related species, M. Forés, M. Duran and M. Solà 234 (1998) 1
- An ab initio study of NMR isotropic shielding bond length derivatives in phosphorus compounds, A. Dransfeld and D.B. Chesnut 234 (1998) 69
- Infrared spectra of polycyclic aromatic hydrocarbons: nitrogen substitution, C.W. Bauschlicher, Jr. 234 (1998) 87
- Tunneling splittings in vibrational spectra of non-rigid molecules: III. Tunneling coordinate-dependent coupling between small amplitude motions, V.A. Benderskii, E.V. Vetoshkin and H.P. Trommsdorff 234 (1998) 153
- Tunneling splittings in vibrational spectra of non-rigid molecules. IV. Kinematic couplings, V.A. Benderskii and E.V. Vetoshkin 234 (1998) 173
- Light induced *cis-trans* isomerization of azo compounds in polymethyl methacrylate, S.Yu. Grebenkin and B.V. Bol'shakov 234 (1998) 239
- Fragmentation pathways in the dissociation of fluoro-iodo-benzene negative ions, R.F.M. Lobo, A.M.C. Moutinho and M.J. Calhorda 234 (1998) 265
- On the role of the energy loss in turnover theories of activated rate processes, A.N. Drozdov and J.J. Brey 235 (1998) 147
- Non-adiabatic effects in condensed phase activated rate processes in the near-adiabatic limit, A.I. Shushin and M. Tachiya 235 (1998) 267

- On the $O_2(v') + O_2(v'')$ atmospheric reaction. II. The role of rotational excitation, W. Wang and A.J.C. Varandas 236 (1998) 181
- Ab-initio CI calculations of the C1s and Cl1s and 2p core excitation spectra of the freon molecules: CCl_4 , $CFCI_3$, CF_2Cl_2 and CF_3Cl , G. Fronzoni and P. Decleva 237 (1998) 21
- Modelling the substitution effects of several rhodium(III) transition metal complexes using the angular overlap model, B. Gilliams, D. Vandenbroucke and C. Görrler-Walrand 237 (1998) 91
- Ab initio study of the electronic spectrum of $C_2H_2^+$. I. Vertical spectrum and angular potential curves, M. Perić, B. Engels and M. Hanrath 238 (1998) 33
- Ab initio study of the electronic spectrum of $C_2H_2^+$. II. Stretching potential energy surfaces for low-lying doublet electronic states, M. Perić and B. Engels 238 (1998) 47
- The first-order electric field-induced spectra: theory and experimental study of NO_2 , J.H. Chen, P.N. Wang, F.M. Li, Y.Q. Chen and Z.G. Wang 238 (1998) 165
- The electronic states of pyrrole studied by optical (VUV) absorption, near-threshold electron energy-loss (EEL) spectroscopy and ab initio multi-reference configuration interaction calculations, M.H. Palmer, I.C. Walker and M.F. Guest 238 (1998) 179
- The study on the magnetic field effect and the microwave effect on the photoconductivity observed in the photolysis of N,N,N',N' -tetramethyl-*p*-phenylenediamine: theoretical calculation trial by the stochastic Liouville equation, Y. Kitahama and H. Murai 238 (1998) 429
- Raman spectroscopy study on the dynamic behavior of nitrate anion in zinc nitrate solution at high temperatures and pressure, Y. Ikushima and M. Arai 238 (1998) 455
- Anion spectroscopy of uracil, thymine and the amino-oxo and amino-hydroxy tautomers of cytosine and their water clusters, J. Schiedt, R. Weinkauff, D.M. Neumark and E.W. Schlag 239 (1998) 511
- Cavitation contribution to the free energy of solvation. Comparison of different formalisms in the context of MST calculations, C. Colominas, F.J. Luque, J. Teixidó and M. Orozco 240 (1999) 253
- A Keilson–Storer type collision kernel for rotation–translation coupling, M.F. Gelin 240 (1999) 265
- Are the changes in the lifetime of the excited uranyl ion of chemical or physical nature?, M. Bouby, I. Billard, A. Bonnenfant and G. Klein 240 (1999) 353
- diatomic*
- High-resolution photoelectron spectroscopy using multibunch synchrotron radiation: rotational-resolved photoelectron bands of $O_2^+(b^4\Sigma_g^-, v^+)$, C.-W. Hsu, M. Evans, S. Stimson, C.Y. Ng and P. Heimann 231 (1998) 121
- Reactions of $N_2^+(v)$ with CO and NO at thermal energy, M.J. Frost, S. Kato, V.M. Bierbaum and S.R. Leone 231 (1998) 145
- Bonding in molecular dications from the classical valence bond viewpoint. A case study of CO^{2+} , R. Polák 232 (1998) 25
- A theoretical study of the electronic structure and spectroscopic properties of the low-lying electronic states of the molecule AlSi, F.R. Ornellas and S. Iwata 232 (1998) 95
- Effect of the angular dependence of the barrier height on the features of the $F + H_2$ reaction, V.M. Azriel, L.Yu. Rusin, M.B. Sevryuk and J.P. Toennies 232 (1998) 307
- Ab initio variational calculation of dynamic polarizabilities and hyperpolarizabilities. I. Polarizability and quadratic hyperpolarizability of water, carbon monoxide and hydrogen fluoride, A. Lembarki, C. Barbier, Ph. Lemaire and E.N. Svendsen 232 (1998) 343
- Polarisation effects in electronically inelastic collisions: $SiFC^2\Delta + H_2 \rightarrow SiFB^2\Sigma^+ + H_2$, N.A. Jackson, C.J. Randall and K.G. McKendrick 233 (1998) 45
- Mechanism of the coherent control of the photoionization and photodissociation of HI and DI, J.A. Fiss, L. Zhu, K. Suto, G. He and R.J. Gordon 233 (1998) 335

- Ab initio study of the $X^2\Sigma^+$ and $A^2\Pi$ states of the SiO^+ cation including the effect of core correlation, Z.-L. Cai and J.P. François 234 (1998) 59
- REMPI spectroscopy of internal state populations in $\text{HBr} + \text{Ar}$ free jets: Rotational relaxation of HBr , A.E. Belikov, M.M. Ahern and M.A. Smith 234 (1998) 195
- Vibrational energy relaxation in liquid oxygen, K.F. Everitt, S.A. Egorov and J.L. Skinner 235 (1998) 115
- A semiclassical study of dissociation dynamics in $\text{He} + \text{H}_2$ collisions, K. Sakimoto 236 (1998) 123
- Rotational alignment from the reactions $\text{Sr}(^3P_J) + \text{CCl}_4$ and CHCl_3 , M.-L. Wang, K.-L. Han, J.-P. Zhan, J.-H. Huang and G.-Z. He 236 (1998) 387
- Vibrationally state-selective laser pulse control of electronic branching in $\text{OH}(X^2\Pi/A^2\Sigma^+)$ photoassociation, M.V. Korolkov and B. Schmidt 237 (1998) 123
- Linear response calculations of electronic g -factors and spin-rotational coupling constants for diatomic molecules with a triplet ground state, M. Engström, B. Minaev, O. Vahtras and H. Ågren 237 (1998) 149
- Theoretical study of the effect of reagent rotation and vibration on the reactions of $\text{Cl} + \text{H}_2$ and $\text{Cl} + \text{HD}$, J.-B. Song and E.A. Gislason 237 (1998) 159
- Charge transfer recombination of Si^{2+} ions from atomic hydrogen, M.C. Bacchus-Montabonel 237 (1998) 245
- A rigorous quantum molecular dynamics study of a collinear $\text{A} + \text{BC} \rightarrow \text{AB} + \text{C}$ reaction, L. Wang 237 (1998) 305
- Quantum study of oriented NO scattering from $\text{Ag}(111)$: orientational steering and effects of surface corrugation, D. Lemoine and T. Duhoo 238 (1998) 59
- A simple analytical estimate of the bound-free Franck–Condon factors for a transition to a repulsive exponential potential in a diatomic molecule, V. Brems 238 (1998) 85
- Threshold photoelectron spectroscopy of HCl and DCl , A.J. Yencha, A.J. Cormack, R.J. Donovan, A. Hopkirk and G.C. King 238 (1998) 109
- Threshold photoelectron spectroscopy of HBr and DBr , A.J. Yencha, A.J. Cormack, R.J. Donovan, K.P. Lawley, A. Hopkirk and G.C. King 238 (1998) 133
- Charge transfer between Si^{3+} and helium at thermal and low energies, P. Honvault, M.C. Bacchus-Montabonel, M. Gargaud and R. McCarroll 238 (1998) 401
- New investigation of the photodissociation of the HBr molecule: total cross-section, anisotropy parameter and dependence of the spin–orbit branching on the ground state vibrational level, B. Pouilly and M. Monnerville 238 (1998) 437
- Effects of complex formation on reactions of oxygen with HCl and Ar-HCl , M.W. Lufaso and A.B. McCoy 239 (1998) 187
- Vibrational excitation of the $\text{C}^3\Pi_u$ state of N_2 by electron impact, G. Poparić, M. Vičić and D.S. Belić 240 (1999) 283
- small polyatomics*
- Monte Carlo calculation of partition functions for straight chain alkanes, J. Gang, M.J. Pilling and S.H. Robertson 231 (1998) 183
- Ultrafast laser control of vibrational dynamics for a two-dimensional model of HONO_2 in the ground electronic state: separation of conformers, control of the bond length, selective preparation of the discrete and the continuum states, M. Oppel and G.K. Paramonov 232 (1998) 111
- Fluorescence lifetime of rovibrational states of h_4 -acetaldehyde and spectra of d_4 -acetaldehyde, S.-H. Jen, T.-J. Hsu and I.-C. Chen 232 (1998) 131
- Pathway approach to ultrafast photochemistry: potential surfaces, conical intersections and isomerizations of small polyenes, W. Fuß, S. Lochbrunner, A.M. Müller, T. Schikarski, W.E. Schmid and S.A. Trushin 232 (1998) 161

- Quantitative studies of the photoabsorption (4.5–488 eV) and photoionization (9–59.5 eV) of methyl iodide using dipole electron impact techniques, T.N. Olney, G. Cooper and C.E. Brion 232 (1998) 211
- Ab initio* study of excited-state intramolecular proton dislocation in salicylic acid, A.L. Sobolewski and W. Domcke 232 (1998) 257
- Ab-initio study of a radiative association mechanism application to the $\text{CH}_3^+ + \text{H}_2$ reaction, D. Talbi and M.C. Bacchus-Montabonel 232 (1998) 267
- Ab initio variational calculation of dynamic polarizabilities and hyperpolarizabilities. I. Polarizability and quadratic hyperpolarizability of water, carbon monoxide and hydrogen fluoride, A. Lembarki, C. Barbier, Ph. Lemaire and E.N. Svendsen 232 (1998) 343
- A He(I) photoelectron spectroscopic study of the \tilde{X}^2A_2' state of NH_3^+ and ND_3^+ . A reanalysis and evidence for the coriolis coupling between the bending ν_2 and ν_4 modes, R. Locht, B. Leyh, K. Hottmann and H. Baumgärtel 233 (1998) 145
- The librational and vibrational spectra of water in natrolite, $\text{Na}_2\text{Al}_2\text{Si}_3\text{O}_{10} \cdot 2\text{H}_2\text{O}$ compared with ab-initio calculations, C.M.B. Line and G.J. Kearley 234 (1998) 207
- Investigation of the CS_2^{2+} dication using threshold photoelectrons coincidence spectroscopy, M. Hochlaf, R.I. Hall, F. Penent, J.H.D. Eland and P. Lablanquie 234 (1998) 249
- Fragment ion yields from CFCl_3 photoexcited in regions of the Cl2p, the Cl1s, and the F1s electron transitions, I.H. Suzuki and N. Saito 234 (1998) 255
- CARS studies of bending states of CO_2 : evidence of collisional rotational transitions with odd ΔJ , A.P. Kouzov, D.N. Kozlov and B. Hemmerling 236 (1998) 15
- Decomposition of perchlorodisiloxane, D. Wichmann and K. Jug 236 (1998) 87
- The mechanism of energy transfer in $\text{H}_2\text{O}-\text{H}_2\text{O}$ collisions – a molecular dynamics simulation, H. Svedung, L.E.B. Börjesson, N. Marković and S. Nordholm 236 (1998) 189
- Femtosecond pump–probe studies of chlorine dioxide photochemistry in water and acetonitrile, M.J. Philpott, S.C. Hayes and P.J. Reid 236 (1998) 207
- Rotational alignment from the reactions $\text{Sr}(^3P_J) + \text{CCl}_4$ and CHCl_3 , M.-L. Wang, K.-L. Han, J.-P. Zhan, J.-H. Huang and G.-Z. He 236 (1998) 387
- The mechanism of the $\text{CH}_3\text{O} + \text{CO}$ reaction and the stability of the CH_3OCO radical, J.S. Francisco 237 (1998) 1
- Ab-initio CI calculations of the Cl1s and Cl1s and 2p core excitation spectra of the freon molecules: CCl_4 , CFCl_3 , CF_2Cl_2 and CF_3Cl , G. Fronzoni and P. Decleva 237 (1998) 21
- Dissociative photoionisation of NO_2 up to 26 eV, J.H.D. Eland and L. Karlsson 237 (1998) 139
- IR–IR double-resonance studies of vibrational relaxation of CD_3F in solid and liquid Xe, Kr, Ar solutions near the melting point, K.S. Rutkowski 237 (1998) 403
- An experimental study of the valence shell photoelectron spectrum of the NO_2 molecule, P. Baltzer, L. Karlsson, B. Wannberg, D.M.P. Holland, M.A. MacDonald, M.A. Hayes and J.H.D. Eland 237 (1998) 451
- An X-ray absorption near edge spectroscopy (XANES) study on organochromium complexes at the Cr K-edge, C. Engemann, J. Hormes, A. Longen and K.H. Dötz 237 (1998) 471
- Vertical double ionization of the sulphur dioxide molecule, I.W. Griffiths, D.E. Parry and F.M. Harris 238 (1998) 21
- On the dielectric continuum solvent model for theoretical estimates of the conformational equilibrium of molecules with an intramolecular hydrogen bond, T. Yasuda and S.-i. Ikawa 238 (1998) 173
- Inner-shell excitation of PF_3 , PCl_3 , PCl_2CF_3 , OPF_3 and SPF_3 . Part I. Spectroscopy, J.J. Neville, A. Jürgensen, R.G. Cavell, N. Kosugi and A.P. Hitchcock 238 (1998) 201

- Multi-photon dissociation of CHBr_3 at 248 and 193 nm: observation of the electronically excited $\text{CH}(\text{A}^2\Delta)$ product, J. Lindner, K. Ermisch and R. Wilhelm 238 (1998) 329
- The vibrational and temperature dependence of the indirect nuclear spin–spin coupling constants of the oxonium (H_3O^+) and hydroxyl (OH^-) ions, S.P.A. Sauer, C.K. Møller, H. Koch, I. Paidarová and V. Špirko 238 (1998) 385
- 'Anomalous' density of states and rotational selection rules of loosely bound states of NO_2 , A. Delon, S. Heilliette and R. Jost 238 (1998) 465
- Infrared photodissociation spectra of isomeric $\text{SiOH}^+-\text{Ar}_n$ ($n = 1-10$) complexes, R.V. Olkhov, S.A. Nizkorodov and O. Dopfer 239 (1998) 393
- Analysis of a nonlinear optical response of CN^- ions adsorbed on metal electrode: tentative interpretation by means of ab initio molecular calculations, M. Tadjeddine and J.P. Flament 240 (1999) 39
- On librational broadening of vibrational transitions in liquids: a simple model, D.J. Ulness, J.C. Kirkwood and A.C. Albrecht 240 (1999) 109
- A semiclassical surface-hopping procedure for vibrational relaxation in polyatomic molecules: model calculations, P. Velez and M.F. Herman 240 (1999) 241
- Absolute photoabsorption oscillator strengths by electron energy loss methods: the valence and S 2p and 2s inner shells of sulphur dioxide in the discrete and continuum regions (3.5–260 eV), R. Feng, G. Cooper, G.R. Burton, C.E. Brion and L. Avaldi 240 (1999) 371
- aromatics*
- Differential ring proton NMR shieldings and cyclic stabilization energies, D.B. Chesnut 231 (1998) 1
- Infrared spectra of polycyclic aromatic hydrocarbons: oxygen substitution, C.W. Bauschlicher, Jr. 233 (1998) 29
- Model study of proton transfer in a H-bonded cluster with an A–H...B reaction complex. Introduction of an effective coordinate for the solvation shell, M.V. Vener 233 (1998) 77
- Instability of self-trapped Frenkel exciton states in one-dimensional microcrystallites, M. Takeshima, J. Singh and A.H. Matsui 233 (1998) 97
- Vibrational coherence in ultrafast electron-transfer dynamics of oxazine 1 in N,N-dimethylaniline: simulation of a femtosecond pump-probe experiment, B. Wolfseder, L. Seidner, W. Domcke, G. Stock, M. Seel, S. Engleitner and W. Zinth 233 (1998) 323
- Ab initio calculations and supersonic jet studies on the geometry of 4-dimethylaminobenzonitrile (DMABN) and related compounds in the ground and excited state, U. Lommatzsch and B. Brutschy 234 (1998) 35
- Infrared spectra of polycyclic aromatic hydrocarbons: methyl substitution and loss of H, C.W. Bauschlicher, Jr. and S.R. Langhoff 234 (1998) 79
- Infrared spectra of polycyclic aromatic hydrocarbons: nitrogen substitution, C.W. Bauschlicher, Jr. 234 (1998) 87
- Valence photoionization of C_6H_6 by the B-spline one-centre expansion density functional method, M. Venuti, M. Stener and P. Decleva 234 (1998) 95
- Fragmentation pathways in the dissociation of fluoro-iodo-benzene negative ions, R.F.M. Lobo, A.M.C. Moutinho and M.J. Calhorda 234 (1998) 265
- Photophysical and lasing properties of pyrromethene 567 dye in liquid solution. Environment effects, F. López Arbeloa, T. López Arbeloa, I. López Arbeloa, I. García-Moreno, A. Costela, R. Sastre and F. Amat-Guerri 236 (1998) 331
- A study of the spectroscopic and thermodynamic properties of furan by means of photoabsorption, photoelectron and photoion spectroscopy, E.E. Rennie, C.A.F. Johnson, J.E. Parker, D.M.P. Holland, D.A. Shaw, M.A. MacDonald, M.A. Hayes and L.G. Shpinkova 236 (1998) 365

- The structure of the lowest excited singlet (S_1) state of 4,4'-bipyridine: a picosecond time-resolved Raman analysis, C. Didierjean, V. De Waele, G. Buntinx and O. Poizat 237 (1998) 169
- Peculiarity of triplet–triplet energy transfer from 2-(2'-hydroxy-phenyl)benzoxazole to diacetyl. Evidence for radiative keto–enol transitions $^3K^* \rightarrow ^1E$ and $^1E \rightarrow ^1K^*$, B. Nickel and P.J. Walla 237 (1998) 371
- Proximity effects in the excited state ordering and photophysics of thienyl-pyridyl ketones, A. Romani, F. Ortica and G. Favaro 237 (1998) 413
- Complexes of spiropyran-derived merocyanines with metal ions: relaxation kinetics, photochemistry and solvent effects, A.K. Chibisov and H. Görner 237 (1998) 425
- On the electronic spectroscopy of benzyl alcohol, J.M. Gingell, G. Marston, N.J. Mason, H. Zhao and M.R.F. Siggel 237 (1998) 443
- Vibrational analysis of 2-nitrophenol. A joint FT-IR, FT-Raman and scaled quantum mechanical study, A. Kovács, V. Izvekov, G. Keresztury and G. Pongor 238 (1998) 231
- Double resonance spectroscopy of phenol(H_2O)_{1–12}: evidence for ice-like structures in aromate–water clusters?, W. Roth, M. Schmitt, Ch. Jacoby, D. Spangenberg, Ch. Janzen and K. Kleinermanns 239 (1998) 1
- Laser-induced fluorescence spectroscopy of van der Waals complexes of tetracene–Ar_N ($N \leq 5$) and pentacene–Ar within ultracold liquid He droplets, M. Hartmann, A. Lindinger, J.P. Toennies and A.F. Vilesov 239 (1998) 139
- ZEKE electron spectroscopy of azulene and azulene–argon, D. Tanaka, S. Sato and K. Kimura 239 (1998) 437
- Ab initio study of the amino group twisting and wagging reaction paths in the intramolecular charge transfer of 4-(N,N-dimethylamino)benzonitrile, W. Sudholt, A.L. Sobolewski and W. Domcke 240 (1999) 9
- other large*
- Intramolecular proton-transfer cycle of 2,4-dimethoxy-6-(1-hydroxy-2-naphthyl)-s-triazine studied by laser photolysis, M. Moriyama, Y. Kawakami, S. Tobita and H. Shizuka 231 (1998) 205
- The vibrational spectroscopy of C₆₀H₃₆: An experimental and theoretical study, R. Bini, J. Ebenhoch, M. Fanti, P.W. Fowler, S. Leach, G. Orlandi, Ch. Rüchardt, J.P.B. Sandall and F. Zerbetto 232 (1998) 75
- Vibrational energy transfer processes in dye molecules after ultrafast excitation of skeletal modes, T. Dahinten, J. Baier and A. Seilmeier 232 (1998) 239
- Wavelength dependence of the nonlinear absorption properties of laser dyes in solid and liquid solutions, J. Barroso, A. Costela, I. García-Moreno and R. Sastre 238 (1998) 257
- Solvent effects within the CS INDO method. Geometrical distortion and solvatochromism of merocyanine dyes, I. Baraldi, F. Momicchioli, G. Ponterini and D. Vanossi 238 (1998) 353
- polymeric and biological*
- Theoretical study of X-ray circular dichroism of amino acids, O. Plashkevych, V. Caravetta, O. Vahtras and H. Ågren 232 (1998) 49
- Low-temperature thermoluminescence in poly(methyl-phenylsilylene), A. Kadashchuk, N. Ostapenko, V. Zaika and S. Nešpůrek 234 (1998) 285
- The electronic structure of poly(pyridine-2,5-diyl) investigated by soft X-ray absorption and emission spectroscopies, M. Magnuson, L. Yang, J.-H. Guo, C. Sâthe, A. Agui, J. Nordgren, Y. Luo, H. Ågren, N. Johansson, W.R. Salaneck, L.E. Horsburgh and A.P. Monkman 237 (1998) 295
- Molecular modelling study for chiral separation of equol enantiomers by β -cyclodextrin, E. Alvira, J.I. García and J.A. Mayoral 240 (1999) 101

- Simulation of excitonic optical line shapes of cyclic molecular aggregates with 9 and 18 units: influence of quasi-static and dynamic disorder, I. Barvík, C. Warns, T. Neidlinger and P. Reineker 240 (1999) 173
- Molecular aggregates*
- Optical limiting properties of a zinc porphyrin polymer and its dimer and monomer model compounds, F.M. Qureshi, S.J. Martin, X. Long, D.D.C. Bradley, F.Z. Henari, W.J. Blau, E.C. Smith, C.H. Wang, A.K. Kar and H.L. Anderson 231 (1998) 87
- Improvement in photoelectric conversion of a phthalocyanine-sensitized TiO₂ electrode by doping with porphyrin, H. Deng, Z. Lu, Y. Shen, H. Mao and H. Xu 231 (1998) 95
- Effect of Al(CO)_x complexation on the aluminum oxidation process, M.J. McQuaid and J.L. Gole 234 (1998) 297
- Quantum hysteresis and resonant tunneling in bistable systems, M. Thorwart, P. Reimann, P. Jung and R.F. Fox 235 (1998) 61
- Effects of non-Markovian relaxation in the femtosecond differential absorption spectra, E. Gaižauskas, A. Beržanskis and K.-H. Feller 235 (1998) 123
- Ab initio study of the equilibrium conformation of the ArCO⁺ ion, K.-M. Weitzel 237 (1998) 43
- Analysis of the reaction paths to dissociation of dichloro-ethylenes into Cl₂ and C₂H₂, S.M. Resende and W.B. De Almeida 238 (1998) 11
- 'Fractional heating' differential scanning calorimetry: a tool to study energetics and kinetics of solid-state reactions in photoactive systems with distributed parameters, J. Sworakowski and S. Nešpůrek 238 (1998) 343
- Vibrational spectroscopy of single methanol molecules attached to liquid water clusters, F. Huisken, S. Mohammad-Pooran and O. Werhahn 239 (1998) 11
- Hydrogen bonding in (substituted benzene) · (water)_n clusters with $n \leq 4$, H.-D. Barth, K. Buchhold, S. Djafari, B. Reimann, U. Lommatzsch and B. Brutschy 239 (1998) 49
- The B ← X spectrum of ArCl₂: linear and perpendicular isomers, K.C. Janda, D. Djahandideh, O. Roncero and N. Halberstadt 239 (1998) 177
- A contribution to the structure determination of Ar–thiophene: the electric dipole moment, U. Spoerel and D. Consalvo 239 (1998) 199
- Infrared photodissociation spectra of isomeric SiOH⁺–Ar_n ($n = 1–10$) complexes, R.V. Olkhov, S.A. Nizkorodov and O. Dopfer 239 (1998) 393
- Photodissociation spectroscopy of (benzene–toluene)⁺. Charge delocalization in the hetero-dimer ion, K. Ohashi, Y. Nakane, Y. Inokuchi, Y. Nakai and N. Nishi 239 (1998) 429
- Improved intermolecular water potential from global geometry optimization of small water clusters using local MP2, B. Hartke, M. Schütz and H.-J. Werner 239 (1998) 561
- dimers*
- Hartree–Fock limit properties of the water dimer in absence of BSSE, A. Famulari, M. Raimondi, M. Sironi and E. Gianinetti 232 (1998) 275
- Ab initio MO–VB study of water dimer, A. Famulari, M. Raimondi, M. Sironi and E. Gianinetti 232 (1998) 289
- A density functional study of weakly bound hydrogen bonded complexes, A.K. Chandra and M.T. Nguyen 232 (1998) 299
- Fifth-order two-dimensional vibrational spectroscopy of a Morse potential system in condensed phases, Y. Tanimura 233 (1998) 217
- ¹⁷O nuclear quadrupole resonance study of proton disorder in solid benzoic acid, 4-hydroxybenzoic acid and 4-nitrobenzoic acid, J. Seliger and V. Žagar 234 (1998) 223

- Interplay of creation, propagation, and relaxation of an excitation in a dimer, J. Peřina, Jr. 236 (1998) 157
- Manifestation of interaction of the transition dipole moments in IR spectra of low-temperature liquids and solutions in liquefied noble gases, T.D. Kolomiitsova, A.P. Burtsev, V.G. Fedoseev and D.N. Shchepkin 238 (1998) 315
- Highly resolved UV spectroscopy of clusters: isotope substitution studies of hydrogen-bonded phenol · water, R.M. Helm and H.J. Neusser 239 (1998) 33
- A contribution to the rotational spectrum, structure, and dynamics of the benzonitrile–water complex in the S_0 electronic state, V. Storm, H. Dreizler and D. Consalvo 239 (1998) 109
- Threshold electron attachment and electron impact ionization involving oxygen dimers, J. Kreil, M.-W. Ruf, H. Hotop, I. Ettischer and U. Buck 239 (1998) 459
- Localisation vs. delocalisation in the dimeric mixed-valence clusters in the generalised vibronic model. Magnetic manifestations, J.J. Borrás-Almenar, E. Coronado, S.M. Ostrovsky, A.V. Palii and B.S. Tsukerblat 240 (1999) 149
- van der Waals molecules*
- Hartree–Fock limit properties of the water dimer in absence of BSSE, A. Famulari, M. Raimondi, M. Sironi and E. Gianinetti 232 (1998) 275
- Ab initio MO–VB study of water dimer, A. Famulari, M. Raimondi, M. Sironi and E. Gianinetti 232 (1998) 289
- Instability of self-trapped Frenkel exciton states in one-dimensional microcrystallites, M. Takeshima, J. Singh and A.H. Matsui 233 (1998) 97
- Structure of the Van der Waals rare gas– C_{60} exohedral complexes $[(C_{60})(RG)_n; n = 1, 2]$, S. Iglesias-Groth, J. Breton and C. Girardet 237 (1998) 285
- Interaction anisotropy and quantum dynamics for vibrationally inelastic collisions of $LiH(^1\Sigma)$ with $He(^1S)$, E. Bodo, E. Buonomo, F.A. Gianturco, S. Kumar, A. Famulari, M. Raimondi and M. Sironi 237 (1998) 315
- Rotational spectra of the ^{15}N -aniline–X, (X = Ar, Ne) complexes. Structure determination from studies on isotopomers, V. Storm, H. Dreizler and D. Consalvo 237 (1998) 395
- Equatorial piperidine and the piperidine–water complex. Rotational spectra and molecular structures, U. Spoerel and W. Stahl 239 (1998) 97
- Effects of complex formation on reactions of oxygen with HCl and Ar–HCl, M.W. Lufaso and A.B. McCoy 239 (1998) 187
- A contribution to the structure determination of Ar–thiophene: the electric dipole moment, U. Spoerel and D. Consalvo 239 (1998) 199
- Electronic spectroscopy and excited state dynamics of the Al– N_2 complex, X. Yang, I. Gerasimov and P.J. Dagdigan 239 (1998) 207
- Adducts of aromatic molecules with rare gases: rotational spectrum of pyrazole–argon, W. Caminati, P.G. Favero and B. Velino 239 (1998) 223
- Rotational spectrum and dynamics of tetrahydrofuran–argon, S. Melandri, J.C. López, P.G. Favero, W. Caminati and J.L. Alonso 239 (1998) 229
- Large-amplitude motion in highly quantum clusters: high-resolution infrared absorption studies of jet-cooled H_2 –HCl and H_2 –DCI, D.T. Anderson, M. Schuder and D.J. Nesbitt 239 (1998) 253
- Ultrafast dynamics of transition metal carbonyls. II. Picosecond evaporation after photodissociation of $Cr(CO)_6 \cdot (CH_3OH)_n$ heteroclusters at 280 nm, M. Gutmann, J.M. Janello and M.S. Dickebohm 239 (1998) 317
- Structure and dynamics of the phenol–water–argon cation radical, D.M. Chapman, F.J. Hompf, K. Müller-Dethlefs, E. Waterstradt, P. Hobza and V. Špirko 239 (1998) 417

- ZEKE electron spectroscopy of azulene and azulene–argon, D. Tanaka, S. Sato and K. Kimura 239 (1998) 437
- Threshold electron attachment and electron impact ionization involving oxygen dimers, J. Kreil, M.-W. Ruf, H. Hotop, I. Ettischer and U. Buck 239 (1998) 459
- Anion spectroscopy of uracil, thymine and the amino-oxo and amino-hydroxy tautomers of cytosine and their water clusters, J. Schiedt, R. Weinkauff, D.M. Neumark and E.W. Schlag 239 (1998) 511
- Competition between electronic and vibrational predissociation in $\text{Ar-I}_2(B)$: a molecular dynamics with quantum transitions study, A. Bastida, J. Zuñiga, A. Requena, N. Halberstadt and J.A. Beswick 240 (1999) 229
- clusters*
- Mode-dependent anharmonic coupling between OH stretching and intermolecular vibrations of the hydrogen-bonded clusters of phenol, T. Ebata, K. Nagao and N. Mikami 231 (1998) 199
- Modelling aluminium clusters with an empirical many-body potential, L.D. Lloyd and R.L. Johnston 236 (1998) 107
- Emission spectra of HeAr_2^+ and HeKr_2^+ heterotrimer ions produced in a helium flowing afterglow, M. Tsuji, M. Tanaka, E. Oda, H. Ishimi and Y. Nishimura 236 (1998) 319
- Classical energy calculations with electron correlation of condensed excited states — Rydberg Matter, L. Holmlid 237 (1998) 11
- Hybrid procedure of the ab initio molecular orbital (MO) method and the Monte Carlo samplings; application to cluster $\text{B}^+(\text{H}_2\text{O})$, H. Watanabe and T. Asada 237 (1998) 81
- On the dependence of a critical supersaturation on pressure of a two-component background gas in a diffusion cloud chamber, A.L. Itkin 238 (1998) 273
- Double resonance spectroscopy of $\text{phenol}(\text{H}_2\text{O})_{1-12}$: evidence for ice-like structures in aromate–water clusters?, W. Roth, M. Schmitt, Ch. Jacoby, D. Spangenberg, Ch. Janzen and K. Kleinerann 239 (1998) 1
- Investigations of OH–N- and NH–O-type hydrogen-bonded clusters by UV laser spectroscopy, C. Jacoby, P. Hering, M. Schmitt, W. Roth and K. Kleinerann 239 (1998) 23
- Hydrogen bonding in (substituted benzene) · (water)_n clusters with $n \leq 4$, H.-D. Barth, K. Buchhold, S. Djafari, B. Reimann, U. Lommatzsch and B. Brutschy 239 (1998) 49
- Electronic spectroscopy of jet-cooled anthracene/(H₂O)_n clusters ($n = 1-16$): comparisons of inhomogeneous structure, P.M. Palmer and M.R. Topp 239 (1998) 65
- Resonant ion-dip infrared spectroscopy of benzene–(water)_n–(methanol)_m clusters with $n + m = 4, 5$, F.C. Hagemeister, C.J. Gruenloh and T.S. Zwierr 239 (1998) 83
- Equatorial piperidine and the piperidine–water complex. Rotational spectra and molecular structures, U. Spoerel and W. Stahl 239 (1998) 97
- On the use of evaporation dynamics to characterize phase transitions in van der Waals clusters: investigations in aniline–(argon)_n up to $n = 15$, P. Parneix, F.G. Amar and P. Bréchnignac 239 (1998) 121
- Laser-induced fluorescence spectroscopy of van der Waals complexes of tetracene–Ar_N ($N \leq 5$) and pentacene–Ar within ultracold liquid He droplets, M. Hartmann, A. Lindinger, J.P. Toennies and A.F. Vilesov 239 (1998) 139
- Existence of two internal energy distributions in jet-formed van der Waals heteroclusters: example of the anthracene–argon_n system, D. Uridat, V. Brenner, I. Dimicoli, J. Le Calvé, P. Millié, M. Mons and F. Piuze 239 (1998) 151
- Penning ionization of C₆₀ and C₇₀, J.M. Weber, K. Hansen, M.-W. Ruf and H. Hotop 239 (1998) 271

- Angular and velocity distributions of small cluster fragments in neutral $(\text{NH}_3)_n$ scattering off LiF(100), C. Menzel, R. Baumfalk and H. Zacharias 239 (1998) 287
- Capture dynamics in collisions between fullerene ions and rare gas atoms, E.E.B. Campbell, R. Ehlich, G. Heusler, O. Knospe and H. Sprang 239 (1998) 299
- Charge stripping effects from highly charged iodine ions formed from Coulomb explosion of CH_3I clusters, L. Poth, Q. Zhong, J.V. Ford, S.M. Hurley and A.W. Castleman Jr. 239 (1998) 309
- Reactivity of vinyl chloride ionic clusters, S. Martrenchard, C. Dedonder-Lardeux, I. Dimicoli, G. Grégoire, C. Jouvet, M. Mons and D. Solgadi 239 (1998) 331
- Vibrational and unimolecular dissociation of mixed solvent cluster ions: $\text{Na}^+((\text{CH}_3)_2\text{CO})_n(\text{CH}_3\text{OH})_m$, C.J. Weinheimer and J.M. Lisy 239 (1998) 357
- Photofragmentation dynamics of the $(\text{N}_2\text{O})_2^+$ and $(\text{N}_2\text{O})_3^+$ clusters: fragment $\text{N}_2\text{O}^+ \text{A} \leftarrow \text{X}$ spectra, S.A. Nizkorodov and E.J. Bieske 239 (1998) 369
- Stability and reactivity of hydrated magnesium cations, C. Berg, M. Beyer, U. Achatz, S. Joos, G. Niedner-Schatteburg and V.E. Bondybey 239 (1998) 379
- High-resolution electron ionization study of CO , $(\text{CO})_2$ and $(\text{CO})_3$: appearance energies and bond dissociation energies, D. Muigg, G. Denifl, A. Stamatovic, O. Echt and T.D. Märk 239 (1998) 409
- Photodissociation of $\text{Mg}^+-(\text{CH}_3\text{OH})_N$ complexes: evidence for the onset of solvation, M.R. France, S.H. Pullins and M.A. Duncan 239 (1998) 447
- Neutral and negatively-charged formamide, N-methylformamide and dimethylformamide clusters, C. Desfrancois, V. Périquet, S. Carles, J.P. Schermann and L. Adamowicz 239 (1998) 475
- Mass-selected "matrix isolation" infrared spectroscopy of the $\text{I}^-(\text{H}_2\text{O})_2$ complex: making and breaking the inter-water hydrogen-bond, P. Ayotte, G.H. Weddle, J. Kim and M.A. Johnson 239 (1998) 485
- Photoelectron-photofragment coincidence studies of the dissociative photodetachment of O_4^- , K.A. Hanold and R.E. Continetti 239 (1998) 493
- Modeling structure and dynamics of solvated molecular ions: Photodissociation and recombination in $\text{I}_2^-(\text{CO}_2)_n$, J. Faeder, N. Delaney, P.E. Maslen and R. Parson 239 (1998) 525
- Calculation of structures and vibrational spectra of acetonitrile clusters, J.G. Siebers, U. Buck and T.A. Beu 239 (1998) 549
- Improved intermolecular water potential from global geometry optimization of small water clusters using local MP2, B. Hartke, M. Schütz and H.-J. Werner 239 (1998) 561
- Many-body exchange effects in clusters of rare gases with a chromophore: He_2CO_2 , J. Jakowski, G. Chałasiński, M.M. Szcześniak and S.M. Cybulski 239 (1998) 573
- Melting behavior of the $(\text{H}_2\text{O})_6$ and $(\text{H}_2\text{O})_8$ clusters, J.M. Pedulla and K.D. Jordan 239 (1998) 593
- L-Alanyl-L-alanine in the zwitterionic state: structures determined in the presence of explicit water molecules and with continuum models using density functional theory, M. Knapp-Mohammady, K.J. Jalkanen, F. Nardi, R.C. Wade and S. Suhai 240 (1999) 63
- High-order double exchange in mixed-valence $[\text{Fe(III)Fe(II)}]$ cluster, M.I. Belinsky 240 (1999) 303
- complexes*
- Improvement in photoelectric conversion of a phthalocyanine-sensitized TiO_2 electrode by doping with porphyrin, H. Deng, Z. Lu, Y. Shen, H. Mao and H. Xu 231 (1998) 95
- Electronic spectroscopy and predissociation mechanism of Ar-NO in the 3p Rydberg states, K. Tsuji, K. Aiuchi, K. Shibuya and K. Obi 231 (1998) 279
- Solvation of chromone using combined Discrete/SCRF models, C. Alemán and S.E. Galembeck 232 (1998) 151

- Effect of $\text{Al}(\text{CO})_x$ complexation on the aluminum oxidation process, M.J. McQuaid and J.L. Gole 234 (1998) 297
- Complete basis set ab initio study of monocomplexation of aluminum with H_2O , NH_3 , and HF, B.S. Jursic 237 (1998) 51
- Infrared spectra and theoretical calculations of HCl complexed with NO, L. Krim and M.E. Alikhani 237 (1998) 265
- Isomeric structures, large amplitude intermolecular motions and electronic relaxation of the propynal–Ar complex, P. DeRose, P.-Y. Cheng, B. Xue, S.-S. Ju and H.-L. Dai 239 (1998) 235
- Mode dependence of the state-to-state vibrational dynamics of HCN–HF, L. Oudejans and R.E. Miller 239 (1998) 345
- DIM models for RgX_2^- systems: suppressed influence of spin-orbit coupling and induced multipole effects for the Ar– I_2^- interaction, F.Y. Naumkin 240 (1999) 79
- Molecular modelling study for chiral separation of equol enantiomers by β -cyclodextrin, E. Alvira, J.I. García and J.A. Mayoral 240 (1999) 101
- Nonlinear absorption and refraction in porphyrazine derivatives, C.Y. Tsai, S.P. Chen and T.C. Wen 240 (1999) 191
- Modeling nonlinear optical properties of inorganic complexes. Counterion effects, T.R. Cundari, H.A. Kurtz and T. Zhou 240 (1999) 205
- Free radicals (incl. hydronium and muonium)*
- Kinetic and mechanistic study of the reaction of atomic chlorine with methyl bromide over an extended temperature range, C.A. Piety, R. Soller, J.M. Nicovich, M.L. McKee and P.H. Wine 231 (1998) 155
- Infrared spectroscopy of the NO_3 radical, K. Kawaguchi, T. Ishiwata, E. Hirota and I. Tanaka 231 (1998) 193
- Uptake coefficient of OH radical on aqueous surface, A. Takami, S. Kato, A. Shimono and S. Koda 231 (1998) 215
- Direct observation of the equilibrium between cyclohexenyl radicals, O_2 , and cyclohexenylperoxy radicals, R. Zils, S. Inomata, Y. Okunuki and N. Washida 231 (1998) 303
- Monte Carlo and molecular orbital study of solvent effect on the electronic structure and hyperfine coupling constants of the $(\text{CH}_3)_2\text{NO}$ radical: the effect of electron transfer between the solute and solvent molecules, T. Yagi, H. Takase, K. Morihashi and O. Kikuchi 232 (1998) 1
- Kinetics of the $\text{CN} + \text{CH}_2\text{CO}$ and $\text{NCO} + \text{CH}_2\text{CO}$ reactions, M.A. Edwards and J.F. Hershberger 234 (1998) 231
- Ultraviolet absorption spectrum and cross-sections of vinyl (C_2H_3) radical in the 225–238 nm region, A. Fahr, P. Hassanzadeh and D.B. Atkinson 236 (1998) 43
- Theoretical study of the ethylene radical cation: geometry and hyperfine structure, N. Salhi-Benachenhou, B. Engels, M.-B. Huang and S. Lunell 236 (1998) 53
- Isotope effect in diffusion of methyl radicals in glassy ethanol-1,2- d_5 at low temperatures, V.L. Vyazovkin and V.A. Tolkmachev 236 (1998) 291
- Positronium formation and quenching in frozen and liquid solutions in octanol, F. Bockstahl, I. Billard, G. Duplâtre and A. Bonnenfant 236 (1998) 393
- The mechanism of the $\text{CH}_3\text{O} + \text{CO}$ reaction and the stability of the CH_3OCO radical, J.S. Francisco 237 (1998) 1
- The electronic structure and Raman spectroscopy of the first purely organic ferromagnet: β para-nitrophenyl nitronyl nitroxide, C. Xiao, K. Feng, Y. Mo, Q. Meng, M. Zhang, M. Wan and J. Zhao 237 (1998) 73

Quasiparticles (incl. excitons)

- Instability of self-trapped Frenkel exciton states in one-dimensional microcrystallites, M. Takeshima, J. Singh and A.H. Matsui 233 (1998) 97
- Role of the local electric field in electro-absorption spectra of molecular crystals, R.W. Munn 236 (1998) 151
- Quantum motion of particles along one-dimensional pathways with static and dynamic energy disorder, L.D.A. Siebbeles and Y.A. Berlin 238 (1998) 97
- Yamanouchi-chain \mathcal{S}_n -invariant hierarchies for SR carrier space of $\{T^k(v)\}(SU2 \times \mathcal{S}_n)$ dual tensors in NMR: some maximal \mathcal{S}_n -inner products, via \mathcal{S}_n -restricted-space Schur Fn. product mappings, F.P. Temme 238 (1998) 245
- Frenkel exciton scattering at microcrystallite surfaces caused by electric dipoles and monopoles, M. Takeshima and A.H. Matsui 240 (1999) 413

Defects and impurities

- Dynamics of structural relaxation upon Rydberg excitation of an impurity in an Ar crystal, S. Jimenez, A. Pasquarello, R. Car and M. Chergui 233 (1998) 343
- Diatomics-in-molecules applied to solid hydrogen doped with $O(^1D_g)$, P.J. Kuntz 240 (1999) 19

Ions and charge carriers

- Franck–Condon effects in low-energy states of $C_{10}H_8^+$ radical. Ab initio MCSCF study of absorption and resonance Raman spectra, T. Andruniow and M. Pawlikowski 236 (1998) 25
- Ab initio study of the equilibrium conformation of the $ArCO^+$ ion, K.-M. Weitzel 237 (1998) 43
- Nonequilibrium dissociation of hydrogen in a parallel-plate radio frequency discharge, S. Longo and I.D. Boyd 238 (1998) 445
- Modeling structure and dynamics of solvated molecular ions: Photodissociation and recombination in $I_2^-(CO_2)_n$, J. Faeder, N. Delaney, P.E. Maslen and R. Parson 239 (1998) 525
- Investigation of vibrational states of the $ArHCl^+$ cation in the electronic ground state, C. Zuhrt, R. Neumann and L. Zülicke 240 (1999) 117
- Hole transport in arylamine doped polymers, S.A. Visser, W.T. Gruenbaum, E.H. Magin and P.M. Borsenberger 240 (1999) 197

Supramolecular assemblies (incl. nanoparticles and nanostructures)

- Modelling aluminium clusters with an empirical many-body potential, L.D. Lloyd and R.L. Johnston 236 (1998) 107
- Simulation of excitonic optical line shapes of cyclic molecular aggregates with 9 and 18 units: influence of quasi-static and dynamic disorder, I. Barvík, C. Warns, T. Neidlinger and P. Reineker 240 (1999) 173

Liquid–liquid and liquid–solid interfaces

- Electrical properties of a charged surface in a general electrolyte solution, Y.-C. Kuo and J.-P. Hsu 236 (1998) 1
- The second-harmonic response of single-crystal silver electrodes obtained with an interference method, G. Beltramo, C. Bilger, B. Pettinger and W. Schmickler 238 (1998) 473

Biological assemblies, cells and organelles

- Optical dephasing in photosynthetic pigment–protein complexes, H. Fidder, G.J.S. Fowler, C.N. Hunter and V. Sundström 233 (1998) 311
- Thermodynamical and mechanical efficiency of a ratchet pump, I.M. Sokolov and A. Blumen 235 (1998) 39
- High-order double exchange in mixed-valence $[Fe(III)Fe(II)]$ cluster, M.I. Belinsky 240 (1999) 303

Proteins

- Vibrational coherence in bacterial reaction centers: spectroscopic characterisation of motions active during primary electron transfer, M.H. Vos, M.R. Jones and J.-L. Martin 233 (1998) 179
- Reaction rates when barriers fluctuate: A singular perturbation approach, P. Reimann, R. Bartussek and P. Hänggi 235 (1998) 11
- Dramatic reduction in fluorescence quantum yield in mutants of Green Fluorescent Protein due to fast internal conversion, A.D. Kummer, C. Kompa, H. Lossau, F. Pöllinger-Dammer, M.E. Michel-Beyerle, C.M. Silva, E.J. Bylina, W.J. Coleman, M.M. Yang and D.C. Youvan 237 (1998) 183
- High-order double exchange in mixed-valence [Fe(III)Fe(II)] cluster, M.I. Belinsky 240 (1999) 303

Nucleic acids

- Recognition and characterization of binding modes of Δ - and Λ -[Ru(phen)₃]²⁺ and Δ - and Λ -[Ru(phen)₂DPPZ]²⁺ by the ²³Na NMR relaxation and binding free energy parameters, F.C. Marincola, M. Casu, G. Saba, A. Lai, P. Lincoln and B. Nordén 236 (1998) 301

Membranes

- Electrical interaction between two spherical particles covered by an ion-penetrable charged membrane, J.-P. Hsu and B.-T. Liu 236 (1998) 63

Phenomena*Molecular structure*

- Differential ring proton NMR shieldings and cyclic stabilization energies, D.B. Chesnut 231 (1998) 1
- High-resolution photoelectron spectroscopy using multibunch synchrotron radiation: rotational-resolved photoelectron bands of O₂⁺(b⁴Σ_g⁻, v⁺), C.-W. Hsu, M. Evans, S. Stimson, C.Y. Ng and P. Heimann 231 (1998) 121
- A density functional study of weakly bound hydrogen bonded complexes, A.K. Chandra and M.T. Nguyen 232 (1998) 299
- Towards quantitative diatomics-in-molecules model for the water molecule, B.L. Grigorenko, A.V. Nemukhin and V.A. Apkarian 232 (1998) 321
- Infrared spectra of polycyclic aromatic hydrocarbons: oxygen substitution, C.W. Bauschlicher, Jr. 233 (1998) 29
- Intramolecular proton transfer in the ground and the two lowest-lying singlet excited states of 1-amino-3-propenal and related species, M. Forés, M. Duran and M. Solà 234 (1998) 1
- An ab initio study of NMR isotropic shielding bond length derivatives in phosphorus compounds, A. Dransfeld and D.B. Chesnut 234 (1998) 69
- Infrared spectra of polycyclic aromatic hydrocarbons: methyl substitution and loss of H, C.W. Bauschlicher, Jr. and S.R. Langhoff 234 (1998) 79
- Infrared spectra of polycyclic aromatic hydrocarbons: nitrogen substitution, C.W. Bauschlicher, Jr. 234 (1998) 87
- Effect of Al(CO)_x complexation on the aluminum oxidation process, M.J. McQuaid and J.L. Gole 234 (1998) 297
- Theoretical study of the ethylene radical cation: geometry and hyperfine structure, N. Salhi-Benachenhou, B. Engels, M.-B. Huang and S. Lunell 236 (1998) 53

- Decomposition of perchlorodisiloxane, D. Wichmann and K. Jug 236 (1998) 87
- Modelling aluminium clusters with an empirical many-body potential, L.D. Lloyd and R.L. Johnston 236 (1998) 107
- Constant temperature simulations using the Langevin equation with velocity Verlet integration, M.G. Paterlini and D.M. Ferguson 236 (1998) 243
- The mechanism of the $\text{CH}_3\text{O} + \text{CO}$ reaction and the stability of the CH_3OCO radical, J.S. Francisco 237 (1998) 1
- Ab initio study of the equilibrium conformation of the ArCO^+ ion, K.-M. Weitzel 237 (1998) 43
- Hybrid procedure of the ab initio molecular orbital (MO) method and the Monte Carlo samplings; application to cluster $\text{B}^+(\text{H}_2\text{O})$, H. Watanabe and T. Asada 237 (1998) 81
- Infrared spectra and theoretical calculations of HCl complexed with NO, L. Krim and M.E. Alikhani 237 (1998) 265
- Rotational spectra of the ^{15}N -aniline-X, (X = Ar, Ne) complexes. Structure determination from studies on isotopomers, V. Storm, H. Dreizler and D. Consalvo 237 (1998) 395
- Analysis of the reaction paths to dissociation of dichloro-ethylenes into Cl_2 and C_2H_2 , S.M. Resende and W.B. De Almeida 238 (1998) 11
- Ab initio study of the electronic spectrum of C_2H_2^+ . I. Vertical spectrum and angular potential curves, M. Perić, B. Engels and M. Hanrath 238 (1998) 33
- Ab initio study of the electronic spectrum of C_2H_2^+ . II. Stretching potential energy surfaces for low-lying doublet electronic states, M. Perić and B. Engels 238 (1998) 47
- On the dielectric continuum solvent model for theoretical estimates of the conformational equilibrium of molecules with an intramolecular hydrogen bond, T. Yasuda and S.-i. Ikawa 238 (1998) 173
- The electronic states of pyrrole studied by optical (VUV) absorption, near-threshold electron energy-loss (EEL) spectroscopy and ab initio multi-reference configuration interaction calculations, M.H. Palmer, I.C. Walker and M.F. Guest 238 (1998) 179
- Mass spectrometric and theoretical study of the mixed complex $\text{NaCeCl}_4(\text{g})$, J. Kapala, S. Roszak, I. Lisek and M. Miller 238 (1998) 221
- Electronic spectroscopy of jet-cooled anthracene/ $(\text{H}_2\text{O})_n$ clusters ($n = 1-16$): comparisons of inhomogeneous structure, P.M. Palmer and M.R. Topp 239 (1998) 65
- Equatorial piperidine and the piperidine–water complex. Rotational spectra and molecular structures, U. Spoerel and W. Stahl 239 (1998) 97
- A contribution to the rotational spectrum, structure, and dynamics of the benzonitrile–water complex in the S_0 electronic state, V. Storm, H. Dreizler and D. Consalvo 239 (1998) 109
- Laser-induced fluorescence spectroscopy of van der Waals complexes of tetracene- Ar_N ($N \leq 5$) and pentacene-Ar within ultracold liquid He droplets, M. Hartmann, A. Lindinger, J.P. Toennies and A.F. Vilesov 239 (1998) 139
- A contribution to the structure determination of Ar–thiophene: the electric dipole moment, U. Spoerel and D. Consalvo 239 (1998) 199
- Adducts of aromatic molecules with rare gases: rotational spectrum of pyrazole–argon, W. Caminati, P.G. Favero and B. Velino 239 (1998) 223
- Rotational spectrum and dynamics of tetrahydrofuran–argon, S. Melandri, J.C. López, P.G. Favero, W. Caminati and J.L. Alonso 239 (1998) 229
- Large-amplitude motion in highly quantum clusters: high-resolution infrared absorption studies of jet-cooled $\text{H}_2\text{--HCl}$ and $\text{H}_2\text{--DCl}$, D.T. Anderson, M. Schuder and D.J. Nesbitt 239 (1998) 253
- Infrared photodissociation spectra of isomeric $\text{SiOH}^+\text{--Ar}_n$ ($n = 1-10$) complexes, R.V. Olkhov, S.A. Nizkorodov and O. Dopfer 239 (1998) 393

- Improved intermolecular water potential from global geometry optimization of small water clusters using local MP2, B. Hartke, M. Schütz and H.-J. Werner 239 (1998) 561
- Infrared absorption and Raman scattering of (Z)-3-hydroxypropenal. A density functional theoretical study, J. Spanget-Larsen 240 (1999) 51
- Molecular modelling study for chiral separation of equol enantiomers by β -cyclodextrin, E. Alvira, J.I. García and J.A. Mayoral 240 (1999) 101
- A gas phase ab initio excited state geometry optimization study of thymine, cytosine and uracil, M.K. Shukla and P.C. Mishra 240 (1999) 319
- Vibrations and rotations of molecules*
- Monte Carlo calculation of partition functions for straight chain alkanes, J. Gang, M.J. Pilling and S.H. Robertson 231 (1998) 183
- Infrared spectroscopy of the NO_3 radical, K. Kawaguchi, T. Ishiwata, E. Hirota and I. Tanaka 231 (1998) 193
- Ultrafast laser control of vibrational dynamics for a two-dimensional model of HONO_2 in the ground electronic state: separation of conformers, control of the bond length, selective preparation of the discrete and the continuum states, M. Oppel and G.K. Paramonov 232 (1998) 111
- Fluorescence lifetime of rovibrational states of h_4 -acetaldehyde and spectra of d_4 -acetaldehyde, S.-H. Jen, T.-J. Hsu and I.-C. Chen 232 (1998) 131
- Dependence of volume-produced H^- ions on the wall recombination probability of H atoms in a low pressure H_2 positive column, J. Loureiro and J. Amorim 232 (1998) 141
- Towards quantitative diatomics-in-molecules model for the water molecule, B.L. Grigorenko, A.V. Nemukhin and V.A. Apkarian 232 (1998) 321
- Infrared spectra of polycyclic aromatic hydrocarbons: oxygen substitution, C.W. Bauschlicher, Jr. 233 (1998) 29
- Transport properties of a reacting gas mixture with strong vibrational and chemical nonequilibrium, E.V. Kustova and E.A. Nagnibeda 233 (1998) 57
- Populations of rotational levels of nitrogen molecules in free jets. Comparison of CARS and electron beam fluorescent technique, R.G. Sharafutdinov, A.A. Ilyukhin, V.V. Smirnov, A.E. Belikov, G.I. Sukhinin and R.L. Pykhov 233 (1998) 127
- Fifth-order two-dimensional vibrational spectroscopy of a Morse potential system in condensed phases, Y. Tanimura 233 (1998) 217
- Quantum time correlation functions and classical coherence, R. Hernandez and G.A. Voth 233 (1998) 243
- Ab initio calculations and supersonic jet studies on the geometry of 4-dimethylamino-benzonitrile (DMABN) and related compounds in the ground and excited state, U. Lommatzsch and B. Brutschy 234 (1998) 35
- Infrared spectra of polycyclic aromatic hydrocarbons: methyl substitution and loss of H, C.W. Bauschlicher, Jr. and S.R. Langhoff 234 (1998) 79
- Infrared spectra of polycyclic aromatic hydrocarbons: nitrogen substitution, C.W. Bauschlicher, Jr. 234 (1998) 87
- The librational and vibrational spectra of water in natrolite, $\text{Na}_2\text{Al}_2\text{Si}_3\text{O}_{10} \cdot 2\text{H}_2\text{O}$ compared with ab-initio calculations, C.M.B. Line and G.J. Kearley 234 (1998) 207
- Investigation of the CS_2^{2+} dication using threshold photoelectrons coincidence spectroscopy, M. Hochlaf, R.I. Hall, F. Penent, J.H.D. Eland and P. Lablanquie 234 (1998) 249
- Vibrational energy relaxation in liquid oxygen, K.F. Everitt, S.A. Egorov and J.L. Skinner 235 (1998) 115
- Vibrational modes in layered double hydroxides and their calcined derivatives, W. Kargunya, R. Baddour-Hadjean, F. Kooli and W. Jones 236 (1998) 225

- Vibrational spectroscopy and molecular dynamics of solvated methanol tetramer and pentamer, D. Meyer zum Büschenfelde and A. Staib 236 (1998) 253
- The mechanism of the $\text{CH}_3\text{O} + \text{CO}$ reaction and the stability of the CH_3OCO radical, J.S. Francisco 237 (1998) 1
- Quantum study of oriented NO scattering from Ag(111): orientational steering and effects of surface corrugation, D. Lemoine and T. Duhoo 238 (1998) 59
- A simple analytical estimate of the bound-free Franck–Condon factors for a transition to a repulsive exponential potential in a diatomic molecule, V. Brems 238 (1998) 85
- The first-order electric field-induced spectra: theory and experimental study of NO_2 , J.H. Chen, P.N. Wang, F.M. Li, Y.Q. Chen and Z.G. Wang 238 (1998) 165
- Vibrational analysis of 2-nitrophenol. A joint FT-IR, FT-Raman and scaled quantum mechanical study, A. Kovács, V. Izvekov, G. Keresztury and G. Pongor 238 (1998) 231
- Rotational tunneling of methyl groups in the hydroquinone/acetonitrile clathrate: A combined deuteron NMR, INS, and computational study, A. Detken, P. Schiebel, M.R. Johnson, H. Zimmermann and U. Haeberlen 238 (1998) 301
- Raman spectroscopy study on the dynamic behavior of nitrate anion in zinc nitrate solution at high temperatures and pressure, Y. Ikushima and M. Arai 238 (1998) 455
- The $\text{B} \leftarrow \text{X}$ spectrum of ArCl_2 : linear and perpendicular isomers, K.C. Janda, D. Djahandideh, O. Roncero and N. Halberstadt 239 (1998) 177
- Adducts of aromatic molecules with rare gases: rotational spectrum of pyrazole–argon, W. Caminati, P.G. Favero and B. Velino 239 (1998) 223
- Rotational spectrum and dynamics of tetrahydrofuran–argon, S. Melandri, J.C. López, P.G. Favero, W. Caminati and J.L. Alonso 239 (1998) 229
- Photofragmentation dynamics of the $(\text{N}_2\text{O})_2^+$ and $(\text{N}_2\text{O})_3^+$ clusters: fragment N_2O^+ $\text{A} \leftarrow \text{X}$ spectra, S.A. Nizkorodov and E.J. Bieske 239 (1998) 369
- Infrared photodissociation spectra of isomeric $\text{SiOH}^+ - \text{Ar}_n$ ($n = 1-10$) complexes, R.V. Olkhov, S.A. Nizkorodov and O. Dopfer 239 (1998) 393
- Structure and dynamics of the phenol–water–argon cation radical, D.M. Chapman, F.J. Hompf, K. Müller-Dethlefs, E. Waterstradt, P. Hobza and V. Špirko 239 (1998) 417
- ZEKE electron spectroscopy of azulene and azulene–argon, D. Tanaka, S. Sato and K. Kimura 239 (1998) 437
- Photodissociation of $\text{Mg}^+ - (\text{CH}_3\text{OH})_N$ complexes: evidence for the onset of solvation, M.R. France, S.H. Pullins and M.A. Duncan 239 (1998) 447
- Mass-selected “matrix isolation” infrared spectroscopy of the $\text{I}^- \cdot (\text{H}_2\text{O})_2$ complex: making and breaking the inter-water hydrogen-bond, P. Ayotte, G.H. Weddle, J. Kim and M.A. Johnson 239 (1998) 485
- Calculation of structures and vibrational spectra of acetonitrile clusters, J.G. Siebers, U. Buck and T.A. Beu 239 (1998) 549
- Analysis of a nonlinear optical response of CN^- ions adsorbed on metal electrode: tentative interpretation by means of ab initio molecular calculations, M. Tadjeddine and J.P. Flament 240 (1999) 39
- Infrared absorption and Raman scattering of (Z)-3-hydroxypropenal. A density functional theoretical study, J. Spanget-Larsen 240 (1999) 51
- On librational broadening of vibrational transitions in liquids: a simple model, D.J. Ulness, J.C. Kirkwood and A.C. Albrecht 240 (1999) 109
- Investigation of vibrational states of the ArHCl^+ cation in the electronic ground state, C. Zuhrt, R. Neumann and L. Zülicke 240 (1999) 117

- Localisation vs. delocalisation in the dimeric mixed-valence clusters in the generalised vibronic model. Magnetic manifestations, J.J. Borrás-Almenar, E. Coronado, S.M. Ostrovsky, A.V. Palii and B.S. Tsukerblat 240 (1999) 149
- Electronic structure and states*
- Quantum chemical modeling of structure and absorption spectra of the chromophore in green fluorescent proteins, A.A. Voityuk, M.-E. Michel-Beyerle and N. Rösch 231 (1998) 13
- C–Br bond rupture in 193 nm photodissociation of vinyl bromide, H. Katayanagi, N. Yonekura and T. Suzuki 231 (1998) 345
- Theoretical study of the Cl 1s and 2p near edge photoabsorption spectra of HCl by accurate ab-initio configuration interaction and density functional approaches, G. Fronzoni, M. Stener, P. Decleva and G. De Alti 232 (1998) 9
- Bonding in molecular dications from the classical valence bond viewpoint. A case study of CO^{2+} , R. Polák 232 (1998) 25
- A Valence-Bond/Hartree–Fock method to determine the Hubbard transfer integrals in organic conductors, F. Castet, L. Ducasse and A. Fritsch 232 (1998) 37
- On the electronic structure of Cu(III) and Ni(III) in $\text{La}_2\text{Li}_{1/2}\text{Cu}_{1/2}\text{O}_4$, $\text{Nd}_2\text{Li}_{1/2}\text{Ni}_{1/2}\text{O}_4$, and Cs_2KCuF_6 , Z. Hu, G. Kaindl, S.A. Warda, D. Reinen, F.M.F. de Groot and B.G. Müller 232 (1998) 63
- Accurate universal basis set for H through Xe for Hartree–Fock calculations, F.E. Jorge and R.F. Martins 233 (1998) 1
- Optimal pump-dump control: phase-locked versus phase-unlocked schemes, Y.J. Yan, Z.W. Shen and Y. Zhao 233 (1998) 191
- Intramolecular proton transfer in the ground and the two lowest-lying singlet excited states of 1-amino-3-propenal and related species, M. Forés, M. Duran and M. Solà 234 (1998) 1
- Ab initio study of the $X^2\Sigma^+$ and $A^2\Pi$ states of the SiO^+ cation including the effect of core correlation, Z.-L. Cai and J.P. François 234 (1998) 59
- Investigation of the CS_2^{2+} dication using threshold photoelectrons coincidence spectroscopy, M. Hochlaf, R.I. Hall, F. Penent, J.H.D. Eland and P. Lablanquie 234 (1998) 249
- Hole trapping in tri-*p*-tolylamine-doped poly(styrene), P.M. Borsenberger, W.T. Gruenbaum, U. Wolf and H. Bässler 234 (1998) 277
- Field-induced localization and nonlinear response of a one-band conductor to a periodic electric field, A.A. Ovchinnikov and K.A. Pronin 235 (1998) 93
- Ultraviolet absorption spectrum and cross-sections of vinyl (C_2H_3) radical in the 225–238 nm region, A. Fahr, P. Hassanzadeh and D.B. Atkinson 236 (1998) 43
- On the electronic energy disposal of calcium excited atom reactions with halogen-containing compounds: Electronic branching ratio and spin–orbit state populations, M. Garay, C.A. Rinaldi, J.M. Orea and A. González Ureña 236 (1998) 343
- A study of the spectroscopic and thermodynamic properties of furan by means of photoabsorption, photoelectron and photoion spectroscopy, E.E. Rennie, C.A.F. Johnson, J.E. Parker, D.M.P. Holland, D.A. Shaw, M.A. MacDonald, M.A. Hayes and L.G. Shpinkova 236 (1998) 365
- Classical energy calculations with electron correlation of condensed excited states — Rydberg Matter, L. Holmlid 237 (1998) 11
- Ab-initio CI calculations of the Cls and ClIs and 2p core excitation spectra of the freon molecules: CCl_4 , CFCl_3 , CF_2Cl_2 and CF_3Cl , G. Fronzoni and P. Decleva 237 (1998) 21
- Theoretical study of the crystal field excitations in CoO, C. de Graaf, W.A. de Jong, R. Broer and W.C. Nieuwpoort 237 (1998) 59

- Model calculations of local exciton levels in the C_{60} fullerene crystals doped with endohedral fullerenes $M@C_{60}$, A. Eilmes and P. Petelenz 237 (1998) 67
- Modelling the substitution effects of several rhodium(III) transition metal complexes using the angular overlap model, B. Gilliams, D. Vandenbroucke and C. Görrler-Walrand 237 (1998) 91
- On the accuracy of averaged relativistic shape-consistent pseudopotentials, L. Maron and C. Teichteil 237 (1998) 105
- The structure of the lowest excited singlet (S_1) state of 4,4'-bipyridine: a picosecond time-resolved Raman analysis, C. Didierjean, V. De Waele, G. Buntinx and O. Poizat 237 (1998) 169
- The electronic structure of poly(pyridine-2,5-diyl) investigated by soft X-ray absorption and emission spectroscopies, M. Magnuson, L. Yang, J.-H. Guo, C. S  the, A. Agui, J. Nordgren, Y. Luo, H.   gren, N. Johansson, W.R. Salaneck, L.E. Horsburgh and A.P. Monkman 237 (1998) 295
- On the electronic spectroscopy of benzyl alcohol, J.M. Gingell, G. Marston, N.J. Mason, H. Zhao and M.R.F. Siggel 237 (1998) 443
- An experimental study of the valence shell photoelectron spectrum of the NO_2 molecule, P. Baltzer, L. Karlsson, B. Wannberg, D.M.P. Holland, M.A. MacDonald, M.A. Hayes and J.H.D. Eland 237 (1998) 451
- An X-ray absorption near edge spectroscopy (XANES) study on organochromium complexes at the Cr K-edge, C. Engemann, J. Hormes, A. Longen and K.H. D  tz 237 (1998) 471
- Complete basis set limit ionization potentials of O_3 and NO_2 using the multiconfigurational spin tensor electron propagator method (MCSTEP), A.J. McKellar, D. Heryadi, D.L. Yeager and J.A. Nichols 238 (1998) 1
- Ab initio study of the electronic spectrum of $C_2H_2^+$. II. Stretching potential energy surfaces for low-lying doublet electronic states, M. Peric   and B. Engels 238 (1998) 47
- Inner-shell excitation of PF_3 , PCl_3 , PCl_2CF_3 , OPF_3 and SPF_3 . Part I. Spectroscopy, J.J. Neville, A. J  rgensen, R.G. Cavell, N. Kosugi and A.P. Hitchcock 238 (1998) 201
- Non-orthogonal orbitals for localized electrons. I. The Spin-Coupled wavefunction, A. Fritsch 238 (1998) 373
- Chemical bonding and magnetic properties of the high-spin molecule $[Mn_{12}O_{12}(HCOO)_{16}(H_2O)_4]$, Y. Duan 238 (1998) 407
- Experimental and theoretical studies of the low-lying electronic states of the simplest benzylic amide [2]catenane, A.M. Brouwer, W.J. Buma, R. Caudano, M. Fanti, C.-A. Fustin, D.A. Leigh, A. Murphy, P. Rudolf, F. Zerbetto and J.M. Zwi  r 238 (1998) 421
- Highly resolved UV spectroscopy of clusters: isotope substitution studies of hydrogen-bonded phenol · water, R.M. Helm and H.J. Neusser 239 (1998) 33
- Isomeric structures, large amplitude intermolecular motions and electronic relaxation of the propynal–Ar complex, P. DeRose, P.-Y. Cheng, B. Xue, S.-S. Ju and H.-L. Dai 239 (1998) 235
- Ab initio study of the amino group twisting and wagging reaction paths in the intramolecular charge transfer of 4-(N,N-dimethylamino)benzonitrile, W. Sudholt, A.L. Sobolewski and W. Domcke 240 (1999) 9
- Diatomics-in-molecules applied to solid hydrogen doped with $O(^1D_g)$, P.J. Kuntz 240 (1999) 19
- DIM models for RgX_2^- systems: suppressed influence of spin-orbit coupling and induced multipole effects for the $Ar-I_2^-$ interaction, F.Y. Naumkin 240 (1999) 79
- Vibrational excitation of the $C^3\Pi_u$ state of N_2 by electron impact, G. Popari  , M. Vi  i   and D.S. Belic   240 (1999) 283
- High-order double exchange in mixed-valence $[Fe(III)Fe(II)]$ cluster, M.I. Belinsky 240 (1999) 303
- Electron paramagnetic resonance of Er^{3+} doped in YVO_4 : hyperfine parameters, S.K. Misra, S. Isber, J.A. Capobianco and E. Cavalli 240 (1999) 313

- A gas phase ab initio excited state geometry optimization study of thymine, cytosine and uracil, M.K. Shukla and P.C. Mishra 240 (1999) 319
- Absolute photoabsorption oscillator strengths by electron energy loss methods: the valence and S 2p and 2s inner shells of sulphur dioxide in the discrete and continuum regions (3.5–260 eV), R. Feng, G. Cooper, G.R. Burton, C.E. Brion and L. Avaldi 240 (1999) 371
- Comparative study of the spectroscopic properties of Cr⁴⁺-doped LiAlO₂ and LiGaO₂, S. Kück and S. Hartung 240 (1999) 387
- Dual fluorescence of the isoquinolinium cation in methanol: time-resolved emission spectra and semiempirical calculations, A.D. Welland, F.W. Schneider and A.B.J. Parusel 240 (1999) 403
- Electric and magnetic properties*
- Solvent effects on NMR spectrum of acetylene calculated by ab initio methods, M. Pecul and J. Sadlej 234 (1998) 111
- Field-induced localization and nonlinear response of a one-band conductor to a periodic electric field, A.A. Ovchinnikov and K.A. Pronin 235 (1998) 93
- Electrical properties of a charged surface in a general electrolyte solution, Y.-C. Kuo and J.-P. Hsu 236 (1998) 1
- Theoretical study of the ethylene radical cation: geometry and hyperfine structure, N. Salhi-Benachenhou, B. Engels, M.-B. Huang and S. Lunell 236 (1998) 53
- Electrical interaction between two spherical particles covered by an ion-penetrable charged membrane, J.-P. Hsu and B.-T. Liu 236 (1998) 63
- A comparative study of the electronic structure of α -MnS (alabandite) calculated at the Hartree-Fock and Density Functional levels of theory, R. Tappero and A. Lichanot 236 (1998) 97
- Electronic structure of planar superconducting systems. From finite to extended model, S. Larsson 236 (1998) 133
- Role of the local electric field in electro-absorption spectra of molecular crystals, R.W. Munn 236 (1998) 151
- The electronic structure and Raman spectroscopy of the first purely organic ferromagnet: β para-nitrophenyl nitronyl nitroxide, C. Xiao, K. Feng, Y. Mo, Q. Meng, M. Zhang, M. Wan and J. Zhao 237 (1998) 73
- The vibrational and temperature dependence of the indirect nuclear spin–spin coupling constants of the oxonium (H₃O⁺) and hydroxyl (OH[−]) ions, S.P.A. Sauer, C.K. Møller, H. Koch, I. Paidarová and V. Špirko 238 (1998) 385
- Chemical bonding and magnetic properties of the high-spin molecule [Mn₁₂O₁₂(HCOO)₁₆(H₂O)₄], Y. Duan 238 (1998) 407
- Radical-substituted allenes as high-spin species and subunits of organic ferromagnets, R. Beust, N. Tyutyulkov, M. Rabinovitz and F. Dietz 240 (1999) 141
- Paramagnetic susceptibility simulations from crystal field effects on Nd³⁺ in magnesium borate MgNd(BO₂)₅, C. Cascales, R. Sáez Puche and P. Porcher 240 (1999) 291
- Spin splittings*
- Linear response calculations of electronic g-factors and spin-rotational coupling constants for diatomic molecules with a triplet ground state, M. Engström, B. Minaev, O. Vahtras and H. Ågren 237 (1998) 149
- High-order double exchange in mixed-valence [Fe(III)Fe(II)] cluster, M.I. Belinsky 240 (1999) 303
- Optical activity*
- Theoretical study of X-ray circular dichroism of amino acids, O. Plashkevych, V. Caravetta, O. Vahtras and H. Ågren 232 (1998) 49

- Ab initio theoretical optical rotations of small molecules, P.L. Polavarapu and D.K. Chakraborty 240 (1999) 1
- Molecular interactions*
- Molecular relaxation in simple dipolar liquids confined between two solid surfaces, S. Senapati and A. Chandra 231 (1998) 65
- Reactions of $N_2^+(v)$ with CO and NO at thermal energy, M.J. Frost, S. Kato, V.M. Bierbaum and S.R. Leone 231 (1998) 145
- A Valence-Bond/Hartree-Fock method to determine the Hubbard transfer integrals in organic conductors, F. Castet, L. Ducasse and A. Fritsch 232 (1998) 37
- Dependence of volume-produced H^- ions on the wall recombination probability of H atoms in a low pressure H_2 positive column, J. Loureiro and J. Amorim 232 (1998) 141
- Hartree-Fock limit properties of the water dimer in absence of BSSE, A. Famulari, M. Raimondi, M. Sironi and E. Gianinetti 232 (1998) 275
- Ab initio MO-VB study of water dimer, A. Famulari, M. Raimondi, M. Sironi and E. Gianinetti 232 (1998) 289
- A density functional study of weakly bound hydrogen bonded complexes, A.K. Chandra and M.T. Nguyen 232 (1998) 299
- Classical and quantum dynamics on the collinear potential energy surface for the reaction of Li with H_2 , N.J. Clarke, M. Sironi, M. Raimondi, S. Kumar, F.A. Gianturco, E. Buonomo and D.L. Cooper 233 (1998) 9
- Instability of self-trapped Frenkel exciton states in one-dimensional microcrystallites, M. Takeshima, J. Singh and A.H. Matsui 233 (1998) 97
- REMPI spectroscopy of internal state populations in $HBr + Ar$ free jets: Rotational relaxation of HBr , A.E. Belikov, M.M. Ahern and M.A. Smith 234 (1998) 195
- Hole trapping in tri-*p*-tolylamine-doped poly(styrene), P.M. Borsenberger, W.T. Gruenbaum, U. Wolf and H. Bässler 234 (1998) 277
- On the $O_2(v') + O_2(v'')$ atmospheric reaction. II. The role of rotational excitation, W. Wang and A.J.C. Varandas 236 (1998) 181
- Analytical theory of time-resolved fluorescence anisotropy and dynamic stokes shift of polar solute molecules based on continuum model for solvent, F. Tanaka and N. Mataga 236 (1998) 277
- Recognition and characterization of binding modes of Δ - and Λ - $[Ru(phen)_3]^{2+}$ and Δ - and Λ - $[Ru(phen)_2DPPZ]^{2+}$ by the ^{23}Na NMR relaxation and binding free energy parameters, F.C. Marincola, M. Casu, G. Saba, A. Lai, P. Lincoln and B. Nordin 236 (1998) 301
- Structure of the Van der Waals rare gas- C_{60} exohedral complexes $[(C_{60})(RG)_n; n = 1, 2]$, S. Iglesias-Groth, J. Breton and C. Girardet 237 (1998) 285
- Dielectric effects of step-increased pressure on the mass- and diffusion-controlled linear chain and network macromolecules growth, D.A. Wasylyshyn and G.P. Johari 237 (1998) 345
- Investigation of spectral diffusion in PMMA on timescales from 10^{-5} to 10^4 seconds via transient and photophysical hole burning, J. Müller, D. Haarer, O.V. Khodykin and B.M. Kharlamov 237 (1998) 483
- Manifestation of interaction of the transition dipole moments in IR spectra of low-temperature liquids and solutions in liquefied noble gases, T.D. Kolomiitsova, A.P. Burtsev, V.G. Fedoseev and D.N. Shchepkin 238 (1998) 315
- New investigation of the photodissociation of the HBr molecule: total cross-section, anisotropy parameter and dependence of the spin-orbit branching on the ground state vibrational level, B. Pouilly and M. Monnerville 238 (1998) 437

- Resonant ion-dip infrared spectroscopy of benzene–(water)_n–(methanol)_m clusters with $n + m = 4, 5$, F.C. Hagemeister, C.J. Gruenloh and T.S. Zwier 239 (1998) 83
- Existence of two internal energy distributions in jet-formed van der Waals heteroclusters: example of the anthracene–argon_n system, D. Uridat, V. Brenner, I. Dimicoli, J. Le Calvé, P. Millié, M. Mons and F. Piuzzi 239 (1998) 151
- Effects of complex formation on reactions of oxygen with HCl and Ar–HCl, M.W. Lufaso and A.B. McCoy 239 (1998) 187
- Electronic spectroscopy and excited state dynamics of the Al–N₂ complex, X. Yang, I. Gerasimov and P.J. Dagdigan 239 (1998) 207
- Large-amplitude motion in highly quantum clusters: high-resolution infrared absorption studies of jet-cooled H₂–HCl and H₂–DCI, D.T. Anderson, M. Schuder and D.J. Nesbitt 239 (1998) 253
- Vibrational and unimolecular dissociation of mixed solvent cluster ions: Na⁺((CH₃)₂CO)_n(CH₃OH)_m, C.J. Weinheimer and J.M. Lisy 239 (1998) 357
- Neutral and negatively-charged formamide, N-methylformamide and dimethylformamide clusters, C. Desfrancois, V. Périquet, S. Carles, J.P. Schermann and L. Adamowicz 239 (1998) 475
- Improved intermolecular water potential from global geometry optimization of small water clusters using local MP2, B. Hartke, M. Schütz and H.-J. Werner 239 (1998) 561
- L-Alanyl-L-alanine in the zwitterionic state: structures determined in the presence of explicit water molecules and with continuum models using density functional theory, M. Knapp-Mohammady, K.J. Jalkanen, F. Nardi, R.C. Wade and S. Suhai 240 (1999) 63
- DIM models for RgX₂[−] systems: suppressed influence of spin-orbit coupling and induced multipole effects for the Ar–I₂[−] interaction, F.Y. Naumkin 240 (1999) 79
- Molecular modelling study for chiral separation of equol enantiomers by β-cyclodextrin, E. Alvira, J.I. García and J.A. Mayoral 240 (1999) 101
- Spectral bandshapes and intensities*
- The vibrational spectroscopy of C₆₀H₃₆: An experimental and theoretical study, R. Bini, J. Ebenhoch, M. Fanti, P.W. Fowler, S. Leach, G. Orlandi, Ch. Rüchardt, J.P.B. Sandall and F. Zerbetto 232 (1998) 75
- A theoretical study of the electronic structure and spectroscopic properties of the low-lying electronic states of the molecule AlSi, F.R. Ornellas and S. Iwata 232 (1998) 95
- Perylene in biphenyl and anthracene crystals: an example of the influence of the host on single-molecule signals, P.J. Walla, F. Jelezko, Ph. Tamarat, B. Lounis and M. Orrit 233 (1998) 117
- A viscoelastic continuum model of non-polar solvation. II. Vibrational dephasing in moderate to high-viscosity liquids and glasses, M.A. Berg and H.W. Hubble 233 (1998) 257
- Population relaxation and non-Markovian frequency fluctuations in third- and fifth-order Raman scattering, T. Steffen and K. Duppen 233 (1998) 267
- CARS studies of bending states of CO₂: evidence of collisional rotational transitions with odd ΔJ , A.P. Kouzov, D.N. Kozlov and B. Hemmerling 236 (1998) 15
- Role of the local electric field in electro-absorption spectra of molecular crystals, R.W. Munn 236 (1998) 151
- Photophysical and lasing properties of pyrromethene 567 dye in liquid solution. Environment effects, F. López Arbeloa, T. López Arbeloa, I. López Arbeloa, I. García-Moreno, A. Costela, R. Sastre and F. Amat-Guerri 236 (1998) 331
- Investigation of spectral diffusion in PMMA on timescales from 10^{−5} to 10⁴ seconds via transient and photophysical hole burning, J. Müller, D. Haarer, O.V. Khodykin and B.M. Kharlamov 237 (1998) 483

- A simple analytical estimate of the bound-free Franck–Condon factors for a transition to a repulsive exponential potential in a diatomic molecule, V. Brems 238 (1998) 85
- On librational broadening of vibrational transitions in liquids: a simple model, D.J. Ulness, J.C. Kirkwood and A.C. Albrecht 240 (1999) 109
- Control of transition state spectra: a variational algorithm, R.T. Skodje, R. Sadeghi and J.L. Krause 240 (1999) 129
- Absolute photoabsorption oscillator strengths by electron energy loss methods: the valence and S 2p and 2s inner shells of sulphur dioxide in the discrete and continuum regions (3.5–260 eV), R. Feng, G. Cooper, G.R. Burton, C.E. Brion and L. Avaldi 240 (1999) 371

Coupling of electronic and nuclear motion

- Spin–orbit branching in the predissociation of the C¹Π state of HCl and DCl: a manifestation of quantum interference, M.H. Alexander, X. Li, R. Liyanage and R.J. Gordon 231 (1998) 331
- C–Br bond rupture in 193 nm photodissociation of vinyl bromide, H. Katayanagi, N. Yonekura and T. Suzuki 231 (1998) 345
- Polarisation effects in electronically inelastic collisions: SiFC²Δ + H₂ → SiFB²Σ⁺ + H₂, N.A. Jackson, C.J. Randall and K.G. McKendrick 233 (1998) 45
- Vibrational coherence in bacterial reaction centers: spectroscopic characterisation of motions active during primary electron transfer, M.H. Vos, M.R. Jones and J.-L. Martin 233 (1998) 179
- Dynamics of structural relaxation upon Rydberg excitation of an impurity in an Ar crystal, S. Jimenez, A. Pasquarello, R. Car and M. Chergui 233 (1998) 343
- An ab initio study of NMR isotropic shielding bond length derivatives in phosphorus compounds, A. Dransfeld and D.B. Chesnut 234 (1998) 69
- Franck–Condon effects in low-energy states of C₁₀H₈⁺ radical. Ab initio MCSCF study of absorption and resonance Raman spectra, T. Andruniow and M. Pawlikowski 236 (1998) 25
- Vibronic coupling effects in the low-energy 1²B_{1g} and 2²B_{1g} states of the C₁₀H₈⁺ radical, T. Andruniow and M. Pawlikowski 236 (1998) 35
- Penning ionization of C₆₀ and C₇₀, J.M. Weber, K. Hansen, M.-W. Ruf and H. Hotop 239 (1998) 271
- Modeling structure and dynamics of solvated molecular ions: Photodissociation and recombination in I₂[−](CO₂)_n, J. Faeder, N. Delaney, P.E. Maslen and R. Parson 239 (1998) 525

Energy transfer processes

- Vibrational energy transfer processes in dye molecules after ultrafast excitation of skeletal modes, T. Dahinten, J. Baier and A. Seilmeier 232 (1998) 239
- Polarisation effects in electronically inelastic collisions: SiFC²Δ + H₂ → SiFB²Σ⁺ + H₂, N.A. Jackson, C.J. Randall and K.G. McKendrick 233 (1998) 45
- Transport properties of a reacting gas mixture with strong vibrational and chemical nonequilibrium, E.V. Kustova and E.A. Nagnibeda 233 (1998) 57
- Optical dephasing in photosynthetic pigment–protein complexes, H. Fidder, G.J.S. Fowler, C.N. Hunter and V. Sundström 233 (1998) 311
- Curvilinear-path based theory of the energy transfer limited rate of a two-dimensional solute in a dissipative bath, S.K. Reese and S.C. Tucker 235 (1998) 171
- On the O₂(v') + O₂(v'') atmospheric reaction. II. The role of rotational excitation, W. Wang and A.J.C. Varandas 236 (1998) 181
- The mechanism of energy transfer in H₂O–H₂O collisions – a molecular dynamics simulation, H. Svedung, L.E.B. Börjesson, N. Marković and S. Nordholm 236 (1998) 189

- Sub-picosecond excited-state dynamics of a carotenoid (spirilloxanthin) in the light-harvesting systems of *Chromatium vinosum*. Relaxation process from the optically allowed S_2 state, H. Okamoto, M. Ogura, T. Nakabayashi and M. Tasumi 236 (1998) 309
- The energy relaxation of Si–H vibration in the H/Si(111) system. Relaxation rate and potential energy surface anharmonicity, V.A. Ermoshin, A.K. Kazansky, K.S. Smirnov and D. Bougeard 237 (1998) 333
- Transport kinetics of triplet excitation in solid chrysene, S.A. Bagnich 237 (1998) 359
- Peculiarity of triplet–triplet energy transfer from 2-(2'-hydroxy-phenyl)benzoxazole to diacetyl. Evidence for radiative keto–enol transitions $^3K^* \rightarrow ^1E$ and $^1E \rightarrow ^1K^*$, B. Nickel and P.J. Walla 237 (1998) 371
- IR–IR double-resonance studies of vibrational relaxation of CD_3F in solid and liquid Xe, Kr, Ar solutions near the melting point, K.S. Rutkowski 237 (1998) 403
- New investigation of the photodissociation of the HBr molecule: total cross-section, anisotropy parameter and dependence of the spin–orbit branching on the ground state vibrational level, B. Pouilly and M. Monnerville 238 (1998) 437
- Nonequilibrium dissociation of hydrogen in a parallel-plate radio frequency discharge, S. Longo and I.D. Boyd 238 (1998) 445
- Angular and velocity distributions of small cluster fragments in neutral $(NH_3)_n$ scattering off LiF(100), C. Menzel, R. Baumfalk and H. Zacharias 239 (1998) 287
- Capture dynamics in collisions between fullerene ions and rare gas atoms, E.E.B. Campbell, R. Ehlich, G. Heusler, O. Knospe and H. Sprang 239 (1998) 299
- Ultrafast dynamics of transition metal carbonyls. II. Picosecond evaporation after photodissociation of $Cr(CO)_6 \cdot (CH_3OH)_n$ heteroclusters at 280 nm, M. Gutmann, J.M. Janello and M.S. Dickebohm 239 (1998) 317
- Mode dependence of the state-to-state vibrational dynamics of HCN–HF, L. Oudejans and R.E. Miller 239 (1998) 345
- Simulation of excitonic optical line shapes of cyclic molecular aggregates with 9 and 18 units: influence of quasi-static and dynamic disorder, I. Barvík, C. Warns, T. Neidlinger and P. Reineker 240 (1999) 173
- Hole transport in arylamine doped polymers, S.A. Visser, W.T. Gruenbaum, E.H. Magin and P.M. Borsenberger 240 (1999) 197
- Are the changes in the lifetime of the excited uranyl ion of chemical or physical nature?, M. Bouby, I. Billard, A. Bonnenfant and G. Klein 240 (1999) 353
- Molecular photophysical processes*
- Improvement in photoelectric conversion of a phthalocyanine-sensitized TiO_2 electrode by doping with porphyrin, H. Deng, Z. Lu, Y. Shen, H. Mao and H. Xu 231 (1998) 95
- Spin–orbit branching in the predissociation of the $C^1\Pi$ state of HCl and DCl: a manifestation of quantum interference, M.H. Alexander, X. Li, R. Liyanage and R.J. Gordon 231 (1998) 331
- Mechanism of the coherent control of the photoionization and photodissociation of HI and DI, J.A. Fiss, L. Zhu, K. Suto, G. He and R.J. Gordon 233 (1998) 335
- Wavepacket diagnosis with chirped probe pulses, R. Zadoyan, N. Schwentner and V.A. Apkarian 233 (1998) 353
- Investigation of the CS_2^{2+} dication using threshold photoelectrons coincidence spectroscopy, M. Hochlaf, R.I. Hall, F. Penent, J.H.D. Eland and P. Lablanquie 234 (1998) 249
- Vibrational energy relaxation in liquid oxygen, K.F. Everitt, S.A. Egorov and J.L. Skinner 235 (1998) 115

- Effects of non-Markovian relaxation in the femtosecond differential absorption spectra, E. Gaižauskas, A. Beržanskis and K.-H. Feller 235 (1998) 123
- Sub-picosecond excited-state dynamics of a carotenoid (spirilloxanthin) in the light-harvesting systems of *Chromatium vinosum*. Relaxation process from the optically allowed S₂ state, H. Okamoto, M. Ogura, T. Nakabayashi and M. Tasumi 236 (1998) 309
- A study of the spectroscopic and thermodynamic properties of furan by means of photoabsorption, photoelectron and photoion spectroscopy, E.E. Rennie, C.A.F. Johnson, J.E. Parker, D.M.P. Holland, D.A. Shaw, M.A. MacDonald, M.A. Hayes and L.G. Shpinkova 236 (1998) 365
- Vibrationally state-selective laser pulse control of electronic branching in OH (X²Π/A²Σ⁺) photoassociation, M.V. Korolkov and B. Schmidt 237 (1998) 123
- Dissociative photoionisation of NO₂ up to 26 eV, J.H.D. Eland and L. Karlsson 237 (1998) 139
- Photogeneration of charge in solid films of α-sexithiophene, J. Kalinowski, W. Stampor, P. Di Marco and F. Garnier 237 (1998) 233
- Proximity effects in the excited state ordering and photophysics of thienyl-pyridyl ketones, A. Romani, F. Ortica and G. Favaro 237 (1998) 413
- An experimental study of the valence shell photoelectron spectrum of the NO₂ molecule, P. Baltzer, L. Karlsson, B. Wannberg, D.M.P. Holland, M.A. MacDonald, M.A. Hayes and J.H.D. Eland 237 (1998) 451
- Investigation of spectral diffusion in PMMA on timescales from 10⁻⁵ to 10⁴ seconds via transient and photophysical hole burning, J. Müller, D. Haarer, O.V. Khodykin and B.M. Kharlamov 237 (1998) 483
- The study on the magnetic field effect and the microwave effect on the photoconductivity observed in the photolysis of N,N,N',N'-tetramethyl-p-phenylenediamine: theoretical calculation trial by the stochastic Liouville equation, Y. Kitahama and H. Murai 238 (1998) 429
- Ab initio study of the amino group twisting and wagging reaction paths in the intramolecular charge transfer of 4-(N,N-dimethylamino)benzonitrile, W. Sudholt, A.L. Sobolewski and W. Domcke 240 (1999) 9

Photochemistry

- Quantum chemical modeling of structure and absorption spectra of the chromophore in green fluorescent proteins, A.A. Voityuk, M.-E. Michel-Beyerle and N. Rösch 231 (1998) 13
- Spin-forbidden dissociation of ozone in the Huggins bands, W. Denzer, G. Hancock, J.C. Pinot de Moira and P.L. Tyley 231 (1998) 109
- Translational energy and angular distributions of O(¹D) and O(³P_j) fragments in the UV photodissociation of ozone, K. Takahashi, N. Taniguchi, Y. Matsumi and M. Kawasaki 231 (1998) 171
- Uptake coefficient of OH radical on aqueous surface, A. Takami, S. Kato, A. Shimono and S. Koda 231 (1998) 215
- Photochemistry of acetone under tropospheric conditions, T. Gierczak, J.B. Burkholder, S. Bauerle and A.R. Ravishankara 231 (1998) 229
- On the UV photodissociation dynamics of hydrogen iodide, S.R. Langford, P.M. Regan, A.J. Orr-Ewing and M.N.R. Ashfold 231 (1998) 245
- New results on the atmospheric photooxidation of simple alkylbenzenes, B. Klotz, I. Barnes and K.H. Becker 231 (1998) 289
- Direct observation of the equilibrium between cyclohexenyl radicals, O₂, and cyclohexenylperoxy radicals, R. Zils, S. Inomata, Y. Okunuki and N. Washida 231 (1998) 303
- C–Br bond rupture in 193 nm photodissociation of vinyl bromide, H. Katayanagi, N. Yonekura and T. Suzuki 231 (1998) 345

- Pathway approach to ultrafast photochemistry: potential surfaces, conical intersections and isomerizations of small polyenes, W. Fuß, S. Lochbrunner, A.M. Müller, T. Schikarski, W.E. Schmid and S.A. Trushin 232 (1998) 161
- Effect of pressure and temperature on the H-atom tunneling in solid phase chemical reactions. The acridine/fluorene system, L.I. Trakhtenberg and V.L. Klochikhin 232 (1998) 175
- Ab initio* study of excited-state intramolecular proton dislocation in salicylic acid, A.L. Sobolewski and W. Domcke 232 (1998) 257
- Intramolecular proton transfer in the ground and the two lowest-lying singlet excited states of 1-amino-3-propenal and related species, M. Forés, M. Duran and M. Solà 234 (1998) 1
- Light induced *cis-trans* isomerization of azo compounds in polymethyl methacrylate, S.Yu. Grebenkin and B.V. Bol'shakov 234 (1998) 239
- Photochemical accumulation and recombination of ion pairs undergoing the singlet-triplet conversion, A.I. Burshtein and A.Yu. Sivachenko 235 (1998) 257
- Femtosecond pump-probe studies of chlorine dioxide photochemistry in water and acetonitrile, M.J. Philpott, S.C. Hayes and P.J. Reid 236 (1998) 207
- Interference-effects in the laser-induced desorption of small molecules from surfaces: a model study, S. Thiel, T. Klüner and H.-J. Freund 236 (1998) 263
- Ultrafast intermolecular electron transfer in coumarin-hydrazine system, H. Shirota, H. Pal, K. Tominaga and K. Yoshihara 236 (1998) 355
- Matrix photochemistry of nitrosyl chloride. Interconversion of ClNO and ClON species by irradiation and tunneling effect, A. Hallou, L. Schriver-Mazzuoli, A. Schriver and P. Chaquin 237 (1998) 251
- Complexes of spiropyran-derived merocyanines with metal ions: relaxation kinetics, photochemistry and solvent effects, A.K. Chibisov and H. Görner 237 (1998) 425
- Multi-photon dissociation of CHBr_3 at 248 and 193 nm: observation of the electronically excited $\text{CH}(\text{A}^2\Delta)$ product, J. Lindner, K. Ermisch and R. Wilhelm 238 (1998) 329
- 'Fractional heating' differential scanning calorimetry: a tool to study energetics and kinetics of solid-state reactions in photoactive systems with distributed parameters, J. Sworakowski and S. Nešpůrek 238 (1998) 343
- Modeling structure and dynamics of solvated molecular ions: Photodissociation and recombination in $\text{I}_2^-(\text{CO}_2)_n$, J. Faeder, N. Delaney, P.E. Maslen and R. Parson 239 (1998) 525
- Intramolecular dynamics*
- A He(I) photoelectron spectroscopic study of the $\tilde{\text{X}}^2\text{A}_2'$ state of NH_3^+ and ND_3^+ . A reanalysis and evidence for the coriolis coupling between the bending ν_2 and ν_4 modes, R. Locht, B. Leyh, K. Hottmann and H. Baumgärtel 233 (1998) 145
- The intermolecular interaction mechanisms in liquid CS_2 at 295 and 165 K probed with two-dimensional Raman spectroscopy, A. Tokmakoff, M.J. Lang, X.J. Jordanides and G.R. Fleming 233 (1998) 231
- ^{17}O nuclear quadrupole resonance study of proton disorder in solid benzoic acid, 4-hydroxybenzoic acid and 4-nitrobenzoic acid, J. Seliger and V. Žagar 234 (1998) 223
- Fragmentation pathways in the dissociation of fluoro-iodo-benzene negative ions, R.F.M. Lobo, A.M.C. Moutinho and M.J. Calhorda 234 (1998) 265
- Effect of $\text{Al}(\text{CO})_x$ complexation on the aluminum oxidation process, M.J. McQuaid and J.L. Gole 234 (1998) 297
- Binary collision theory for thermal and nonisothermal relaxation and reaction of polyatomic molecules, P. Talkner, E. Pollak and A.M. Berezhkovskii 235 (1998) 131
- 'Anomalous' density of states and rotational selection rules of loosely bound states of NO_2 , A. Delon, S. Heilliette and R. Jost 238 (1998) 465

-radiationless transitions

- Optical limiting properties of a zinc porphyrin polymer and its dimer and monomer model compounds, F.M. Qureshi, S.J. Martin, X. Long, D.D.C. Bradley, F.Z. Henari, W.J. Blau, E.C. Smith, C.H. Wang, A.K. Kar and H.L. Anderson 231 (1998) 87
- Dramatic reduction in fluorescence quantum yield in mutants of Green Fluorescent Protein due to fast internal conversion, A.D. Kummer, C. Kompa, H. Lossau, F. Pöllinger-Dammer, M.E. Michel-Beyerle, C.M. Silva, E.J. Bylina, W.J. Coleman, M.M. Yang and D.C. Youvan 237 (1998) 183

-vibrational energy redistribution (incl. vibrational dissociation)

- Optical limiting properties of a zinc porphyrin polymer and its dimer and monomer model compounds, F.M. Qureshi, S.J. Martin, X. Long, D.D.C. Bradley, F.Z. Henari, W.J. Blau, E.C. Smith, C.H. Wang, A.K. Kar and H.L. Anderson 231 (1998) 87
- Reactions of $N_2^+(v)$ with CO and NO at thermal energy, M.J. Frost, S. Kato, V.M. Bierbaum and S.R. Leone 231 (1998) 145
- Vibrational energy transfer processes in dye molecules after ultrafast excitation of skeletal modes, T. Dahinten, J. Baier and A. Seilmeier 232 (1998) 239
- Controlling condensed-phase vibrational excitation with tailored infrared pulses, V.D. Kleiman, S.M. Arrivo, J.S. Melinger and E.J. Heilweil 233 (1998) 207
- Nonadiabatic reactions in condensed phase in the absence of thermal equilibrium, I. Rips 235 (1998) 243
- Competition between electronic and vibrational predissociation in $Ar-I_2(B)$: a molecular dynamics with quantum transitions study, A. Bastida, J. Zuñiga, A. Requena, N. Halberstadt and J.A. Beswick 240 (1999) 229
- A semiclassical surface-hopping procedure for vibrational relaxation in polyatomic molecules: model calculations, P. Velez and M.F. Herman 240 (1999) 241

Luminescence spectra, yields and lifetimes

- Low-temperature thermoluminescence in poly(methyl-phenylsilylene), A. Kadashchuk, N. Ostapenko, V. Zaika and S. Nešpùrek 234 (1998) 285
- Photophysical and lasing properties of pyrromethene 567 dye in liquid solution. Environment effects, F. López Arbeloa, T. López Arbeloa, I. López Arbeloa, I. García-Moreno, A. Costela, R. Sastre and F. Amat-Guerri 236 (1998) 331
- Ultrafast intermolecular electron transfer in coumarin–hydrazine system, H. Shirota, H. Pal, K. Tominaga and K. Yoshihara 236 (1998) 355
- Rotational alignment from the reactions $Sr(^3P_J) + CCl_4$ and $CHCl_3$, M.-L. Wang, K.-L. Han, J.-P. Zhan, J.-H. Huang and G.-Z. He 236 (1998) 387
- Proximity effects in the excited state ordering and photophysics of thienyl-pyridyl ketones, A. Romani, F. Ortica and G. Favaro 237 (1998) 413
- Complexes of spiropyran-derived merocyanines with metal ions: relaxation kinetics, photochemistry and solvent effects, A.K. Chibisov and H. Görner 237 (1998) 425
- Rotational alignment from the $Sr(^3P_J) + CH_2ClI$ chemiluminescent reaction, M.-L. Wang, K.-L. Han, S.-L. Cong, G.-Z. He and N.-Q. Lou 238 (1998) 481
- Paramagnetic susceptibility simulations from crystal field effects on Nd^{3+} in magnesium borate $MgNd(BO_2)_5$, C. Cascales, R. Sáez Puche and P. Porcher 240 (1999) 291
- Are the changes in the lifetime of the excited uranyl ion of chemical or physical nature?, M. Bouby, I. Billard, A. Bonnenfant and G. Klein 240 (1999) 353
- Comparative study of the spectroscopic properties of Cr^{4+} -doped $LiAlO_2$ and $LiGaO_2$, S. Kück and S. Hartung 240 (1999) 387

- Frenkel exciton scattering at microcrystallite surfaces caused by electric dipoles and monopoles, M. Takeshima and A.H. Matsui 240 (1999) 413
- Coherence loss processes*
- Heterodyne-detected stimulated photon echo: applications to optical dynamics in solution, W.P. de Boeij, M.S. Pshenichnikov and D.A. Wiersma 233 (1998) 287
- Optical dephasing in photosynthetic pigment–protein complexes, H. Fidder, G.J.S. Fowler, C.N. Hunter and V. Sundström 233 (1998) 311
- Yamanouchi-chain \mathcal{S}_n -invariant hierarchies for SR carrier space of $\{T^k(v)\}(SU2 \times \mathcal{S}_n)$ dual tensors in NMR: some maximal \mathcal{S}_n -inner products, via \mathcal{S}_n -restricted-space Schur Fn. product mappings, F.P. Temme 238 (1998) 245
- Nonlinear responses (incl. optical)*
- Optical limiting properties of a zinc porphyrin polymer and its dimer and monomer model compounds, F.M. Qureshi, S.J. Martin, X. Long, D.D.C. Bradley, F.Z. Henari, W.J. Blau, E.C. Smith, C.H. Wang, A.K. Kar and H.L. Anderson 231 (1998) 87
- Ab initio variational calculation of dynamic polarizabilities and hyperpolarizabilities. I. Polarizability and quadratic hyperpolarizability of water, carbon monoxide and hydrogen fluoride, A. Lembarki, C. Barbier, Ph. Lemaire and E.N. Svendsen 232 (1998) 343
- Population relaxation and non-Markovian frequency fluctuations in third- and fifth-order Raman scattering, T. Steffen and K. Duppen 233 (1998) 267
- Heterodyne-detected stimulated photon echo: applications to optical dynamics in solution, W.P. de Boeij, M.S. Pshenichnikov and D.A. Wiersma 233 (1998) 287
- Quantum hysteresis and resonant tunneling in bistable systems, M. Thorwart, P. Reimann, P. Jung and R.F. Fox 235 (1998) 61
- An ab initio time-dependent Hartree–Fock study of solvent effects on the polarizability and second hyperpolarizability of polyacetylene chains within the polarizable continuum model, B. Champagne, B. Mennucci, M. Cossi, R. Cammi and J. Tomasi 238 (1998) 153
- Wavelength dependence of the nonlinear absorption properties of laser dyes in solid and liquid solutions, J. Barroso, A. Costela, I. García-Moreno and R. Sastre 238 (1998) 257
- Nonlinear absorption and refraction in porphyrazine derivatives, C.Y. Tsai, S.P. Chen and T.C. Wen 240 (1999) 191
- Modeling nonlinear optical properties of inorganic complexes. Counterion effects, T.R. Cundari, H.A. Kurtz and T. Zhou 240 (1999) 205
- Multiphoton phenomena*
- Coulomb explosion dynamics of N_2 in intense laser field by mass-resolved momentum imaging, A. Hishikawa, A. Iwamae, K. Hoshina, M. Kono and K. Yamanouchi 231 (1998) 315
- Ultrafast laser control of vibrational dynamics for a two-dimensional model of $HONO_2$ in the ground electronic state: separation of conformers, control of the bond length, selective preparation of the discrete and the continuum states, M. Oppel and G.K. Paramonov 232 (1998) 111
- Controlling condensed-phase vibrational excitation with tailored infrared pulses, V.D. Kleiman, S.M. Arrivo, J.S. Melinger and E.J. Heilweil 233 (1998) 207
- Mechanism of the coherent control of the photoionization and photodissociation of HI and DI, J.A. Fiss, L. Zhu, K. Suto, G. He and R.J. Gordon 233 (1998) 335
- Vibrationally state-selective laser pulse control of electronic branching in $OH(X^2\Pi/A^2\Sigma^+)$ photoassociation, M.V. Korolkov and B. Schmidt 237 (1998) 123

Reactions (incl. dissociation)

- Theoretical study of the OH + NO₂ reaction: formation of nitric acid and the hydroperoxyl radical, D. Chakraborty, J. Park and M.C. Lin 231 (1998) 39
- Kinetic and mechanistic study of the reaction of atomic chlorine with methyl bromide over an extended temperature range, C.A. Piety, R. Soller, J.M. Nicovich, M.L. McKee and P.H. Wine 231 (1998) 155
- Uptake coefficient of OH radical on aqueous surface, A. Takami, S. Kato, A. Shimono and S. Koda 231 (1998) 215
- Photochemistry of acetone under tropospheric conditions, T. Gierczak, J.B. Burkholder, S. Bauerle and A.R. Ravishankara 231 (1998) 229
- On the UV photodissociation dynamics of hydrogen iodide, S.R. Langford, P.M. Regan, A.J. Orr-Ewing and M.N.R. Ashfold 231 (1998) 245
- A crossed molecular beam investigation of the reaction Cl + propane → HCl + C₃H₇ using VUV synchrotron radiation as a product probe, D.A. Blank, N. Hemmi, A.G. Suits and Y.T. Lee 231 (1998) 261
- Electronic spectroscopy and predissociation mechanism of Ar–NO in the 3p Rydberg states, K. Tsuji, K. Aiuchi, K. Shibuya and K. Obi 231 (1998) 279
- Classical and quantum dynamics on the collinear potential energy surface for the reaction of Li with H₂, N.J. Clarke, M. Sironi, M. Raimondi, S. Kumar, F.A. Gianturco, E. Buonomo and D.L. Cooper 233 (1998) 9
- Femtosecond photodissociation of triiodide in solution: Excitation energy dependence and transition state dynamics, T. Kühne, R. Küster and P. Vöhringer 233 (1998) 161
- Kinetics of the CN + CH₂CO and NCO + CH₂CO reactions, M.A. Edwards and J.F. Hershberger 234 (1998) 231
- Thermal decay of a metastable elastic string, C. Cattuto, M. Borromeo and F. Marchesoni 235 (1998) 51
- Curvilinear-path based theory of the energy transfer limited rate of a two-dimensional solute in a dissipative bath, S.K. Reese and S.C. Tucker 235 (1998) 171
- Non-adiabatic effects in condensed phase activated rate processes in the near-adiabatic limit, A.I. Shushin and M. Tachiya 235 (1998) 267
- Interplay of creation, propagation, and relaxation of an excitation in a dimer, J. Peřina, Jr. 236 (1998) 157
- On the electronic energy disposal of calcium excited atom reactions with halogen-containing compounds: Electronic branching ratio and spin–orbit state populations, M. Garay, C.A. Rinaldi, J.M. Orea and A. González Ureña 236 (1998) 343
- Theoretical study of the effect of reagent rotation and vibration on the reactions of Cl + H₂ and Cl + HD, J.-B. Song and E.A. Gislason 237 (1998) 159
- Reactions of C(¹D) with H₂, HD and D₂: kinetic isotope effect and the CD/CH branching ratio, K. Sato, N. Ishida, T. Kurakata, A. Iwasaki and S. Tsunashima 237 (1998) 195
- Reactions of solid glycine induced by keV ion irradiation, W. Huang, Z. Yu and Y. Zhang 237 (1998) 223
- Analysis of the reaction paths to dissociation of dichloro-ethylenes into Cl₂ and C₂H₂, S.M. Resende and W.B. De Almeida 238 (1998) 11
- Semiclassical reactive scattering: the Hermite correction method in hyperspherical coordinates, S. Adhikari and G.D. Billing 238 (1998) 69
- Multi-photon dissociation of CHBr₃ at 248 and 193 nm: observation of the electronically excited CH(A²Δ) product, J. Lindner, K. Ermisch and R. Wilhelm 238 (1998) 329
- Rotational alignment from the Sr(³P_J) + CH₂ClI chemiluminescent reaction, M.-L. Wang, K.-L. Han, S.-L. Cong, G.-Z. He and N.-Q. Lou 238 (1998) 481
- Effects of complex formation on reactions of oxygen with HCl and Ar–HCl, M.W. Lufaso and A.B. McCoy 239 (1998) 187

- Capture dynamics in collisions between fullerene ions and rare gas atoms, E.E.B. Campbell, R. Ehlich, G. Heusler, O. Knospe and H. Sprang 239 (1998) 299
- Reactivity of vinyl chloride ionic clusters, S. Martrenchard, C. Dedonder-Lardeux, I. Dimicoli, G. Grégoire, C. Jouvet, M. Mons and D. Solgadi 239 (1998) 331
- Stability and reactivity of hydrated magnesium cations, C. Berg, M. Beyer, U. Achatz, S. Joos, G. Niedner-Schatteburg and V.E. Bondybey 239 (1998) 379
- Photoelectron–photofragment coincidence studies of the dissociative photodetachment of O_4^- , K.A. Hanold and R.E. Continetti 239 (1998) 493
- On the nonequilibrium effects in thermally activated reactions $A + A \rightleftharpoons B + B \rightleftharpoons C + C$, J. Gorecki and J.N. Gorecka 240 (1999) 215
- Contributions to the spectroscopic–kinetic analysis of linear reaction systems. Systems with three linearly independent reactions using the concept of parallel projection, J. Polster 240 (1999) 331
- isolated molecules*
- Spin–orbit branching in the predissociation of the $C^1\Pi$ state of HCl and DCl: a manifestation of quantum interference, M.H. Alexander, X. Li, R. Liyanage and R.J. Gordon 231 (1998) 331
- Laser photodissociation of ketene at 230 nm, M. Castillejo, S. Couris, E. Lane, M. Martin and J. Ruiz 232 (1998) 353
- Mechanism of the coherent control of the photoionization and photodissociation of HI and DI, J.A. Fiss, L. Zhu, K. Suto, G. He and R.J. Gordon 233 (1998) 335
- Fragment ion yields from $CFCl_3$ photoexcited in regions of the $Cl2p$, the $C1s$, and the $F1s$ electron transitions, I.H. Suzuki and N. Saito 234 (1998) 255
- A simple analytical estimate of the bound-free Franck–Condon factors for a transition to a repulsive exponential potential in a diatomic molecule, V. Brems 238 (1998) 85
- ‘Anomalous’ density of states and rotational selection rules of loosely bound states of NO_2 , A. Delon, S. Heilliette and R. Jost 238 (1998) 465
- collisional*
- Photochemistry of acetone under tropospheric conditions, T. Gierczak, J.B. Burkholder, S. Bauerle and A.R. Ravishankara 231 (1998) 229
- Effect of the angular dependence of the barrier height on the features of the $F + H_2$ reaction, V.M. Azriel, L.Yu. Rusin, M.B. Sevryuk and J.P. Toennies 232 (1998) 307
- Transport properties of a reacting gas mixture with strong vibrational and chemical nonequilibrium, E.V. Kustova and E.A. Nagnibeda 233 (1998) 57
- Binary collision theory for thermal and nonisothermal relaxation and reaction of polyatomic molecules, P. Talkner, E. Pollak and A.M. Berezhkovskii 235 (1998) 131
- A semiclassical study of dissociation dynamics in $He + H_2$ collisions, K. Sakimoto 236 (1998) 123
- On the $O_2(v') + O_2(v'')$ atmospheric reaction. II. The role of rotational excitation, W. Wang and A.J.C. Varandas 236 (1998) 181
- Emission spectra of $HeAr_2^+$ and $HeKr_2^+$ heterotrimer ions produced in a helium flowing afterglow, M. Tsuji, M. Tanaka, E. Oda, H. Ishimi and Y. Nishimura 236 (1998) 319
- Rotational alignment from the reactions $Sr(^3P_J) + CCl_4$ and $CHCl_3$, M.-L. Wang, K.-L. Han, J.-P. Zhan, J.-H. Huang and G.-Z. He 236 (1998) 387
- Vibrationally state-selective laser pulse control of electronic branching in $OH(X^2\Pi/A^2\Sigma^+)$ photoassociation, M.V. Korolkov and B. Schmidt 237 (1998) 123
- Theoretical study of the effect of reagent rotation and vibration on the reactions of $Cl + H_2$ and $Cl + HD$, J.-B. Song and E.A. Gislason 237 (1998) 159

- A rigorous quantum molecular dynamics study of a collinear $A + BC \rightarrow AB + C$ reaction, L. Wang 237 (1998) 305
- Interaction anisotropy and quantum dynamics for vibrationally inelastic collisions of $\text{LiH}(^1\Sigma)$ with $\text{He}(^1S)$, E. Bodo, E. Buonomo, F.A. Gianturco, S. Kumar, A. Famulari, M. Raimondi and M. Sironi 237 (1998) 315
- Capture dynamics in collisions between fullerene ions and rare gas atoms, E.E.B. Campbell, R. Ehlich, G. Heusler, O. Knospe and H. Sprang 239 (1998) 299
- condensed phase*
- Curvilinear-path based theory of the energy transfer limited rate of a two-dimensional solute in a dissipative bath, S.K. Reese and S.C. Tucker 235 (1998) 171
- Reversible chemical reactions in slowly relaxing environments: Kramers' turnover of the rate constant, A.M. Berezhkovskii, V.Yu. Zitserman, D.-Y. Yang and S.H. Lin 235 (1998) 201
- Phase space distribution function approach to the Kramers problem. III. Anharmonic potentials, J. Morelli and D.J. Tannor 235 (1998) 213
- Nonadiabatic reactions in condensed phase in the absence of thermal equilibrium, I. Rips 235 (1998) 243
- Non-equilibrium interlevel transitions in condensed phase far away from the avoided crossing region, M.V. Basilevsky, A.V. Soudackov and A.I. Voronin 235 (1998) 281
- Solvent effects on outersphere electron transfer reactions in mixed dipolar liquids, A. Chandra 238 (1998) 285
- Diatomics-in-molecules applied to solid hydrogen doped with $\text{O}(^1D_g)$, P.J. Kuntz 240 (1999) 19
- Effect of solvent fluctuations on proton transfer dynamics: a hybrid AM1/MM molecular dynamics simulation on the $[\text{H}_3\text{N}-\text{H}-\text{NH}_3]^+$ system, G.-S. Li, M.T.C. Martins Costa, C. Millot and M.F. Ruiz-López 240 (1999) 93
- Tunneling*
- Effect of pressure and temperature on the H-atom tunneling in solid phase chemical reactions. The acridine/fluorene system, L.I. Trakhtenberg and V.L. Klochikhin 232 (1998) 175
- Quantum time correlation functions and classical coherence, R. Hernandez and G.A. Voth 233 (1998) 243
- Tunneling splittings in vibrational spectra of non-rigid molecules: III. Tunneling coordinate-dependent coupling between small amplitude motions, V.A. Bendetskii, E.V. Vetoshkin and H.P. Trommsdorff 234 (1998) 153
- Tunneling splittings in vibrational spectra of non-rigid molecules. IV. Kinematic couplings, V.A. Bendetskii and E.V. Vetoshkin 234 (1998) 173
- High frequency satellites in resonant activation, E. Turlot, S. Linkwitz, D. Esteve, C. Urbina, M.H. Devoret and H. Grabert 235 (1998) 47
- Quantum hysteresis and resonant tunneling in bistable systems, M. Thorwart, P. Reimann, P. Jung and R.F. Fox 235 (1998) 61
- Suppression of quantum coherence: Noise effect, J. Shao, C. Zerbe and P. Hänggi 235 (1998) 81
- Non-equilibrium interlevel transitions in condensed phase far away from the avoided crossing region, M.V. Basilevsky, A.V. Soudackov and A.I. Voronin 235 (1998) 281
- Matrix photochemistry of nitrosyl chloride. Interconversion of CINO and ClON species by irradiation and tunneling effect, A. Hallou, L. Schriver-Mazzuoli, A. Schriver and P. Chaquin 237 (1998) 251
- A rigorous quantum molecular dynamics study of a collinear $A + BC \rightarrow AB + C$ reaction, L. Wang 237 (1998) 305
- Rotational tunneling of methyl groups in the hydroquinone/acetonitrile clathrate: A combined deuteron NMR, INS, and computational study, A. Detken, P. Schiebel, M.R. Johnson, H. Zimmermann and U. Haeberlen 238 (1998) 301

- Laser driven hydrogen tunneling in a dissipative environment, H. Naundorf, K. Sundermann and O. Kühn 240 (1999) 163
- Electron transfer*
- Improvement in photoelectric conversion of a phthalocyanine-sensitized TiO₂ electrode by doping with porphyrin, H. Deng, Z. Lu, Y. Shen, H. Mao and H. Xu 231 (1998) 95
- Monte Carlo and molecular orbital study of solvent effect on the electronic structure and hyperfine coupling constants of the (CH₃)₂NO radical: the effect of electron transfer between the solute and solvent molecules, T. Yagi, H. Takase, K. Morihashi and O. Kikuchi 232 (1998) 1
- Quantitative studies of the photoabsorption (4.5–488 eV) and photoionization (9–59.5 eV) of methyl iodide using dipole electron impact techniques, T.N. Olney, G. Cooper and C.E. Brion 232 (1998) 211
- Bridged-assisted electron transfer. Random matrix theory approach, E. Gudowska-Nowak, G. Papp and J. Brickmann 232 (1998) 247
- Charge transfer in gas–surface scattering: the three electronic state system, D. Guan, X. Yi, S. Ding, L. Gu and J.A. Olson 233 (1998) 35
- Vibrational coherence in bacterial reaction centers: spectroscopic characterisation of motions active during primary electron transfer, M.H. Vos, M.R. Jones and J.-L. Martin 233 (1998) 179
- Vibrational coherence in ultrafast electron-transfer dynamics of oxazine 1 in N,N-dimethylaniline: simulation of a femtosecond pump-probe experiment, B. Wolfseder, L. Seidner, W. Domcke, G. Stock, M. Seel, S. Engleitner and W. Zinth 233 (1998) 323
- The steady-state Green's function theory in monomolecular reactions. II. Effects of solvent dynamics and non-equilibrium initial distributions in reactions on position-dependent transition regions, O.B. Jenkins and A.B. Doktorov 234 (1998) 121
- Fragmentation pathways in the dissociation of fluoro-iodo-benzene negative ions, R.F.M. Lobo, A.M.C. Moutinho and M.J. Calhorda 234 (1998) 265
- Photochemical accumulation and recombination of ion pairs undergoing the singlet–triplet conversion, A.I. Burshtein and A.Yu. Sivachenko 235 (1998) 257
- Non-adiabatic effects in condensed phase activated rate processes in the near-adiabatic limit, A.I. Shushin and M. Tachiya 235 (1998) 267
- Ultrafast intermolecular electron transfer in coumarin–hydrazine system, H. Shirota, H. Pal, K. Tominaga and K. Yoshihara 236 (1998) 355
- Photogeneration of charge in solid films of α -sexithiophene, J. Kalinowski, W. Stampor, P. Di Marco and F. Garnier 237 (1998) 233
- Charge transfer recombination of Si²⁺ ions from atomic hydrogen, M.C. Bacchus-Montabonel 237 (1998) 245
- Quantum motion of particles along one-dimensional pathways with static and dynamic energy disorder, L.D.A. Siebbeles and Y.A. Berlin 238 (1998) 97
- Solvent effects on outersphere electron transfer reactions in mixed dipolar liquids, A. Chandra 238 (1998) 285
- Solvent effects within the CS INDO method. Geometrical distortion and solvatochromism of merocyanine dyes, I. Baraldi, F. Momicchioli, G. Ponterini and D. Vanossi 238 (1998) 353
- Cold photoconductivity in a system of interacting charge-transfer excitons at a donor–acceptor interface, S.A. Kiselev, E. Hartung, Z.G. Soos, S.R. Forrest and V.M. Agranovich 238 (1998) 365
- Charge transfer between Si³⁺ and helium at thermal and low energies, P. Honvault, M.C. Bacchus-Montabonel, M. Gargaud and R. McCarroll 238 (1998) 401

- Threshold electron attachment and electron impact ionization involving oxygen dimers, J. Kreil, M.-W. Ruf, H. Hotop, I. Ettischer and U. Buck 239 (1998) 459
- Ab initio study of the amino group twisting and wagging reaction paths in the intramolecular charge transfer of 4-(N,N-dimethylamino)benzonitrile, W. Sudholt, A.L. Sobolewski and W. Domcke 240 (1999) 9
- High-order double exchange in mixed-valence [Fe(III)Fe(II)] cluster, M.I. Belinsky 240 (1999) 303

Proton and hydrogen atom transfer

- Quantum chemical modeling of structure and absorption spectra of the chromophore in green fluorescent proteins, A.A. Voityuk, M.-E. Michel-Beyerle and N. Rösch 231 (1998) 13
- Intramolecular proton-transfer cycle of 2,4-dimethoxy-6-(1-hydroxy-2-naphthyl)-s-triazine studied by laser photolysis, M. Moriyama, Y. Kawakami, S. Tobita and H. Shizuka 231 (1998) 205
- Effect of pressure and temperature on the H-atom tunneling in solid phase chemical reactions. The acridine/fluorene system, L.I. Trakhtenberg and V.L. Klochikhin 232 (1998) 175
- Ab initio study of excited-state intramolecular proton dislocation in salicylic acid, A.L. Sobolewski and W. Domcke 232 (1998) 257
- Model study of proton transfer in a H-bonded cluster with an A–H...B reaction complex. Introduction of an effective coordinate for the solvation shell, M.V. Vener 233 (1998) 77
- Intramolecular proton transfer in the ground and the two lowest-lying singlet excited states of 1-amino-3-propenal and related species, M. Forés, M. Duran and M. Solà 234 (1998) 1
- The steady-state Green's function theory in monomolecular reactions. II. Effects of solvent dynamics and non-equilibrium initial distributions in reactions on position-dependent transition regions, O.B. Jenkins and A.B. Doktorov 234 (1998) 121
- Isotope effect in diffusion of methyl radicals in glassy ethanol-1,2-*d*₅ at low temperatures, V.L. Vyazovkin and V.A. Tolkmachev 236 (1998) 291
- The structure of the lowest excited singlet (*S*₁) state of 4,4'-bipyridine: a picosecond time-resolved Raman analysis, C. Didierjean, V. De Waele, G. Buntinx and O. Poizat 237 (1998) 169
- Dramatic reduction in fluorescence quantum yield in mutants of Green Fluorescent Protein due to fast internal conversion, A.D. Kummer, C. Kompa, H. Lossau, F. Pöllinger-Dammer, M.E. Michel-Beyerle, C.M. Silva, E.J. Bylina, W.J. Coleman, M.M. Yang and D.C. Youvan 237 (1998) 183
- A rigorous quantum molecular dynamics study of a collinear A + BC → AB + C reaction, L. Wang 237 (1998) 305
- Peculiarity of triplet–triplet energy transfer from 2-(2'-hydroxy-phenyl)benzoxazole to diacetyl. Evidence for radiative keto–enol transitions ³K* → ¹E and ¹E → ¹K*, B. Nickel and P.J. Walla 237 (1998) 371
- Infrared absorption and Raman scattering of (Z)-3-hydroxypropenal. A density functional theoretical study, J. Spanget-Larsen 240 (1999) 51
- L-Alanyl-L-alanine in the zwitterionic state: structures determined in the presence of explicit water molecules and with continuum models using density functional theory, M. Knapp-Mohammady, K.J. Jalkanen, F. Nardi, R.C. Wade and S. Suhai 240 (1999) 63
- Effect of solvent fluctuations on proton transfer dynamics: a hybrid AM1/MM molecular dynamics simulation on the [H₃N–H–NH₃]⁺ system, G.-S. Li, M.T.C. Martins Costa, C. Millot and M.F. Ruiz-López 240 (1999) 93
- Laser driven hydrogen tunneling in a dissipative environment, H. Naundorf, K. Sundermann and O. Kühn 240 (1999) 163

Positron annihilation

- Study of positronium hydride with a simple wavefunction: Application to the Stark effect of PsH, C. Le Sech and B. Silvi 236 (1998) 77
- Positronium formation and quenching in frozen and liquid solutions in octanol, F. Bockstahl, I. Billard, G. Duplâtre and A. Bonnenfant 236 (1998) 393
- An experimental test on the distribution of positronium lifetimes in polymers, G. Consolati, R. Rurali and M. Stefanetti 237 (1998) 493

Ionization (incl. Rydberg states)

- Generalization of the Arrhenius relation and ionization reaction rates for carbon atoms and ions in plasmas, Y. Chang and C.A. Ordonez 231 (1998) 27
- Theoretical study of X-ray circular dichroism of amino acids, O. Plashkevych, V. Caravetta, O. Vahtras and H. Ågren 232 (1998) 49
- A He(I) photoelectron spectroscopic study of the $\tilde{X}^2A''_2$ state of NH_3^+ and ND_3^+ . A reanalysis and evidence for the coriolis coupling between the bending ν_2 and ν_4 modes, R. Locht, B. Leyh, K. Hottmann and H. Baumgärtel 233 (1998) 145
- Valence photoionization of C_6H_6 by the B-spline one-centre expansion density functional method, M. Venuti, M. Stener and P. Decleva 234 (1998) 95
- Fragment ion yields from $CFCl_3$ photoexcited in regions of the Cl2p, the Cl1s, and the F1s electron transitions, I.H. Suzuki and N. Saito 234 (1998) 255
- A study of the spectroscopic and thermodynamic properties of furan by means of photoabsorption, photoelectron and photoion spectroscopy, E.E. Rennie, C.A.F. Johnson, J.E. Parker, D.M.P. Holland, D.A. Shaw, M.A. MacDonald, M.A. Hayes and L.G. Shpinkova 236 (1998) 365
- Vertical double ionization of the sulphur dioxide molecule, I.W. Griffiths, D.E. Parry and F.M. Harris 238 (1998) 21
- Threshold photoelectron spectroscopy of HCl and DCl, A.J. Yench, A.J. Cormack, R.J. Donovan, A. Hopkirk and G.C. King 238 (1998) 109
- Threshold photoelectron spectroscopy of HBr and DBr, A.J. Yench, A.J. Cormack, R.J. Donovan, K.P. Lawley, A. Hopkirk and G.C. King 238 (1998) 133
- Penning ionization of C_{60} and C_{70} , J.M. Weber, K. Hansen, M.-W. Ruf and H. Hotop 239 (1998) 271
- High-resolution electron ionization study of CO, $(CO)_2$ and $(CO)_3$: appearance energies and bond dissociation energies, D. Muigg, G. Denifl, A. Stamatovic, O. Echt and T.D. Märk 239 (1998) 409
- ZEKE electron spectroscopy of azulene and azulene-argon, D. Tanaka, S. Sato and K. Kimura 239 (1998) 437
- Threshold electron attachment and electron impact ionization involving oxygen dimers, J. Kreil, M.-W. Ruf, H. Hotop, I. Ettischer and U. Buck 239 (1998) 459
- Anion spectroscopy of uracil, thymine and the amino-oxo and amino-hydroxy tautomers of cytosine and their water clusters, J. Schiedt, R. Weinkauff, D.M. Neumark and E.W. Schlag 239 (1998) 511

Molecular motion (incl. diffusive)

- ^{13}C NMR relaxation in neutral and charged tetra-*n*-alkyl compounds, B. Bordes, F. Coletta, A. Ferrarini, F. Gottardi and P.L. Nordio 231 (1998) 51
- Molecular relaxation in simple dipolar liquids confined between two solid surfaces, S. Senapati and A. Chandra 231 (1998) 65

- Thermodynamical and mechanical efficiency of a ratchet pump, I.M. Sokolov and A. Blumen 235 (1998) 39
- Saddle point avoidance due to inhomogeneous friction, G.J. Moro and F. Cardin 235 (1998) 189
- Numerical simulations of solvation in simple polar fluids: dependence on the thermodynamic state below and above the critical point, P. Graf and A. Nitzan 235 (1998) 297
- A diffusive model for interpreting solvation dynamics in isotropic and ordered liquid phases, A. Polimeno, G. Saielli and P.L. Nordio 235 (1998) 313
- Analytical theory of time-resolved fluorescence anisotropy and dynamic Stokes shift of polar solute molecules based on continuum model for solvent, F. Tanaka and N. Mataga 236 (1998) 277
- Isotope effect in diffusion of methyl radicals in glassy ethanol-1,2- d_5 at low temperatures, V.L. Vyazovkin and V.A. Tolmachev 236 (1998) 291
- Rotational relaxation of perylene in *n*-alcohols and *n*-alkanes studied by two-photon-induced anisotropy decay, S.W. Pauls, J.F. Hedstrom and C.K. Johnson 237 (1998) 205
- Dielectric effects of step-increased pressure on the mass- and diffusion-controlled linear chain and network macromolecules growth, D.A. Wasylyshyn and G.P. Johari 237 (1998) 345
- A Keilson–Storer type collision kernel for rotation–translation coupling, M.F. Gelin 240 (1999) 265
- Isotopic effects*
- Quantitative studies of the photoabsorption (4.5–488 eV) and photoionization (9–59.5 eV) of methyl iodide using dipole electron impact techniques, T.N. Olney, G. Cooper and C.E. Brion 232 (1998) 211
- Isotope effect in diffusion of methyl radicals in glassy ethanol-1,2- d_5 at low temperatures, V.L. Vyazovkin and V.A. Tolmachev 236 (1998) 291
- Threshold photoelectron spectroscopy of HCl and DCl, A.J. Yencha, A.J. Cormack, R.J. Donovan, A. Hopkirk and G.C. King 238 (1998) 109
- Threshold photoelectron spectroscopy of HBr and DBr, A.J. Yencha, A.J. Cormack, R.J. Donovan, K.P. Lawley, A. Hopkirk and G.C. King 238 (1998) 133
- Volume phase transition of polymer gel in water and heavy water, H. Shirota, N. Endo and K. Horie 238 (1998) 487
- Fluctuations and noise*
- Reaction rates when barriers fluctuate: A singular perturbation approach, P. Reimann, R. Bartussek and P. Hänggi 235 (1998) 11
- Brownian transport controlled by dichotomic and thermal fluctuations, J. Kula, M. Kostur and J. Łuczka 235 (1998) 27
- On the role of the energy loss in turnover theories of activated rate processes, A.N. Drozdov and J.J. Brey 235 (1998) 147
- The Kramers problem in 2D-coupled periodic potentials, G. Caratti, R. Ferrando, R. Spadacini and G.E. Tommei 235 (1998) 157
- Reversible chemical reactions in slowly relaxing environments: Kramers' turnover of the rate constant, A.M. Berezhkovskii, V.Yu. Zitserman, D.-Y. Yang and S.H. Lin 235 (1998) 201
- Where is the exit point?, Z. Schuss and A. Spivak 235 (1998) 227
- Surface chemical physics*
- Uptake coefficient of OH radical on aqueous surface, A. Takami, S. Kato, A. Shimono and S. Koda 231 (1998) 215
- Impedance spectroscopic investigation of the temperature influence on the transfer of tetraphenylborate ions through lipid membranes — Calculation of energy barriers for the ion transfer across lipid membranes, K.-D. Schulze 238 (1998) 495

- Vibrational spectroscopy of single methanol molecules attached to liquid water clusters, F. Huisken, S. Mohammad-Pooran and O. Werhahn 239 (1998) 11
- surface scattering*
- The correlation between the statistical properties of surface defect distribution and the specular intensity obtained from low energy He scattering technique, G. Petrella, L. Cassidei and F. Ciriaco 231 (1998) 31
- Quantum study of oriented NO scattering from Ag(111): orientational steering and effects of surface corrugation, D. Lemoine and T. Duhoo 238 (1998) 59
- Angular and velocity distributions of small cluster fragments in neutral $(\text{NH}_3)_n$ scattering off LiF(100), C. Menzel, R. Baumfalk and H. Zacharias 239 (1998) 287
- adsorption*
- Ultraviolet absorption spectrum and cross-sections of vinyl (C_2H_3) radical in the 225–238 nm region, A. Fahr, P. Hassanzadeh and D.B. Atkinson 236 (1998) 43
- desorption*
- Interference-effects in the laser-induced desorption of small molecules from surfaces: a model study, S. Thiel, T. Klüner and H.-J. Freund 236 (1998) 263
- surface excitations*
- The energy relaxation of Si–H vibration in the H/Si(111) system. Relaxation rate and potential energy surface anharmonicity, V.A. Ermoshin, A.K. Kazansky, K.S. Smirnov and D. Bougeard 237 (1998) 333
- adsorbate structure*
- The correlation between the statistical properties of surface defect distribution and the specular intensity obtained from low energy He scattering technique, G. Petrella, L. Cassidei and F. Ciriaco 231 (1998) 31
- surface reactions*
- Charge transfer in gas–surface scattering: the three electronic state system, D. Guan, X. Yi, S. Ding, L. Gu and J.A. Olson 233 (1998) 35
- catalysis*
- Vibrational spectroscopy and molecular dynamics of solvated methanol tetramer and pentamer, D. Meyer zum Büschenfelde and A. Staib 236 (1998) 253
- Electronic process in gases*
- Effect of $\text{Al}(\text{CO})_x$ complexation on the aluminum oxidation process, M.J. McQuaid and J.L. Gole 234 (1998) 297
- Photodissociation spectroscopy of (benzene–toluene) $^+$. Charge delocalization in the hetero-dimer ion, K. Ohashi, Y. Nakane, Y. Inokuchi, Y. Nakai and N. Nishi 239 (1998) 429
- Threshold electron attachment and electron impact ionization involving oxygen dimers, J. Kreil, M.-W. Ruf, H. Hotop, I. Ettischer and U. Buck 239 (1998) 459
- Many-body exchange effects in clusters of rare gases with a chromophore: He_2CO_2 , J. Jakowski, G. Chałasiński, M.M. Szczeniński and S.M. Cybulski 239 (1998) 573

Thermodynamic and transport properties

- Free energies of solvation for peptides and polypeptides using SCRF methods, C. Alemán, H.M. Ishiki, E.A. Armelin, O. Abrahão Junior and S.E. Galembeck 233 (1998) 85
- Thermodynamical and mechanical efficiency of a ratchet pump, I.M. Sokolov and A. Blumen 235 (1998) 39
- Electrical properties of a charged surface in a general electrolyte solution, Y.-C. Kuo and J.-P. Hsu 236 (1998) 1
- Constant temperature simulations using the Langevin equation with velocity Verlet integration, M.G. Paterlini and D.M. Ferguson 236 (1998) 243
- Mass spectrometric and theoretical study of the mixed complex $\text{NaCeCl}_4(\text{g})$, J. Kapala, S. Roszak, I. Lisek and M. Miller 238 (1998) 221
- On the dependence of a critical supersaturation on pressure of a two-component background gas in a diffusion cloud chamber, A.L. Itkin 238 (1998) 273
- 'Fractional heating' differential scanning calorimetry: a tool to study energetics and kinetics of solid-state reactions in photoactive systems with distributed parameters, J. Sworakowski and S. Nešpůrek 238 (1998) 343
- Impedance spectroscopic investigation of the temperature influence on the transfer of tetraphenylborate ions through lipid membranes — Calculation of energy barriers for the ion transfer across lipid membranes, K.-D. Schulze 238 (1998) 495
- Charge stripping effects from highly charged iodine ions formed from Coulomb explosion of CH_3I clusters, L. Poth, Q. Zhong, J.V. Ford, S.M. Hurley and A.W. Castleman Jr. 239 (1998) 309
- Melting behavior of the $(\text{H}_2\text{O})_6$ and $(\text{H}_2\text{O})_8$ clusters, J.M. Pedulla and K.D. Jordan 239 (1998) 593

Structure of solids, liquids and glasses

- Molecular relaxation in simple dipolar liquids confined between two solid surfaces, S. Senapati and A. Chandra 231 (1998) 65
- ^{17}O quadrupole coupling in $\text{C}-\text{O}-\text{H} \cdots \text{O}=\text{C}$ hydrogen bonds, J. Seliger 231 (1998) 81
- Water anomalies and the double-well Takahashi model, C.H. Cho, S. Singh and G.W. Robinson 232 (1998) 329
- Molecular dynamics studies of NaCl solutions in methanol–water mixtures. An effect of NaCl on hydrogen bonded network, E. Hawlicka and D. Swiatla-Wojcik 232 (1998) 361
- An intermolecular potential function for Na^+ –acetonitrile obtained from ab initio calculations. Application to liquid simulations, E.M. Cabaleiro-Lago and M.A. Ríos 236 (1998) 235
- Classical energy calculations with electron correlation of condensed excited states — Rydberg Matter, L. Holmlid 237 (1998) 11
- Paramagnetic susceptibility simulations from crystal field effects on Nd^{3+} in magnesium borate $\text{MgNd}(\text{BO}_2)_5$, C. Cascales, R. Sáez Puche and P. Porcher 240 (1999) 291

Critical behavior and phase transitions

- Positronium formation and quenching in frozen and liquid solutions in octanol, F. Bockstahl, I. Billard, G. Duplâtre and A. Bonnenfant 236 (1998) 393
- On the dependence of a critical supersaturation on pressure of a two-component background gas in a diffusion cloud chamber, A.L. Itkin 238 (1998) 273
- Volume phase transition of polymer gel in water and heavy water, H. Shirota, N. Endo and K. Horie 238 (1998) 487
- On the use of evaporation dynamics to characterize phase transitions in van der Waals clusters: investigations in aniline–(argon) $_n$ up to $n = 15$, P. Parneix, F.G. Amar and P. Bréchnignac 239 (1998) 121

- Melting behavior of the $(\text{H}_2\text{O})_6$ and $(\text{H}_2\text{O})_8$ clusters, J.M. Pedulla and K.D. Jordan 239 (1998) 593
- Cavitation contribution to the free energy of solvation. Comparison of different formalisms in the context of MST calculations, C. Colominas, F.J. Luque, J. Teixidó and M. Orozco 240 (1999) 253
- Electric field effect on the upper critical solution temperature, K. Orzechowski 240 (1999) 275
- Molecular self-assembly and -organization*
- Improvement in photoelectric conversion of a phthalocyanine-sensitized TiO_2 electrode by doping with porphyrin, H. Deng, Z. Lu, Y. Shen, H. Mao and H. Xu 231 (1998) 95
- Vibrational modes in layered double hydroxides and their calcined derivatives, W. Kargunya, R. Baddour-Hadjean, F. Kooli and W. Jones 236 (1998) 225
- An intermolecular potential function for Na^+ -acetonitrile obtained from ab initio calculations. Application to liquid simulations, E.M. Cabaleiro-Lago and M.A. Ríos 236 (1998) 235
- Mass-selected "matrix isolation" infrared spectroscopy of the $\text{I}^- \cdot (\text{H}_2\text{O})_2$ complex: making and breaking the inter-water hydrogen-bond, P. Ayotte, G.H. Weddle, J. Kim and M.A. Johnson 239 (1998) 485

(continued from inside front cover)

Submission of papers: All papers should be submitted in *quadruplicate* to one of the editors.

Electronic manuscripts: Electronic manuscripts have the advantage that there is no need for the rekeying of text, thereby avoiding the possibility of introducing errors and resulting in reliable and fast delivery of proofs.

For the initial submission of manuscripts for consideration, hardcopies are sufficient. For the processing of *accepted papers*, electronic versions are preferred. After *final acceptance*, your disk plus one final and exactly matching printed version should be submitted together. Double density (DD) or high density (HD) diskettes (3.5 or 5.25 inch) are acceptable. It is important that the file saved is in the native format of the wordprocessor program used. Label the disk with the name of the computer and wordprocessing package used, your name, and the name of the file on the disk.

Important: please adhere to instructions to authors, to be found on the last pages of each volume. The instructions can also be found on the World Wide Web: access under <http://www.elsevier.nl> or <http://www.elsevier.com>.

Proofs and reprints: Authors will receive **proofs**, which they are requested to correct and return as soon as possible. No new material may be inserted in the text at the time of proofreading. A total of **50 reprints** of each paper will be supplied free of charge to the author(s). Additional reprints can be ordered at prices shown on the reprint order form.

All questions arising after acceptance of the manuscript, especially those relating to proofs, should be directed to *Chemical Physics*, Elsevier Science B.V., P.O. Box 2759, 1000 CT Amsterdam, The Netherlands. Tel. (+31-20)4852-800, Fax (+31-20)4852-775, E-mail: e.hovens@elsevier.nl

Authors in Japan please note: Upon request, Elsevier Science K.K. will provide authors with a list of people who can check and improve the English of their paper (*before submission*). Please contact our Tokyo office: Elsevier Science K.K., 9-15 Higashi-Azabu, 1-chome Minato-ku, Tokyo 106-0044, Tel. (03)-5561-5032; Fax (03)-5561-5045.

Chemical Physics has no page charges.

Publication information. *Chemical Physics* (ISSN 0301-0104). For 1999 volumes 240–251 are scheduled for publication. Subscription prices are available upon request from the publisher. Subscriptions are accepted on a prepaid basis only and are entered on a calendar year basis. Issues are sent by surface mail except to the following countries where air delivery via SAL is ensured: Argentina, Australia, Brazil, Canada, Hong Kong, India, Israel, Japan, Malaysia, Mexico, New Zealand, Pakistan, PR China, Singapore, South Africa, South Korea, Taiwan, Thailand, USA. For all other countries airmail rates are available upon request. Claims for missing issues must be made within six months of our publication (mailing) date.

Orders, claims, and product enquiries: please contact the Customer Support Department at the Regional Sales Office nearest to you:

New York: Elsevier Science, P.O. Box 945, New York, NY 10159-0945, USA; phone: (+1) (212) 633-3730 [toll free number for North American customers: 1-888-4ES-INFO (437-4636)]; fax: (+1) (212) 633-3680; e-mail: usinfo-f@elsevier.com

Amsterdam: Elsevier Science, P.O. Box 211, 1000 AE Amsterdam, The Netherlands; phone: (+31) 20 4853757; fax: (+31) 20 4853432; e-mail: nlinfo-f@elsevier.nl

Tokyo: Elsevier Science, 9-15 Higashi-Azabu 1-chome, Minato-ku, Tokyo 106-0044, Japan; phone: (+81) (3) 5561 5033; fax: (+81) (3) 5561 5047; e-mail: info@elsevier.co.jp

Singapore: Elsevier Science, No. 1 Temasek Avenue, #17-01 Millenia Tower, Singapore 039192; phone: (+65) 434 3727; fax: (+65) 337 2230; e-mail: asiainfo@elsevier.com.sg

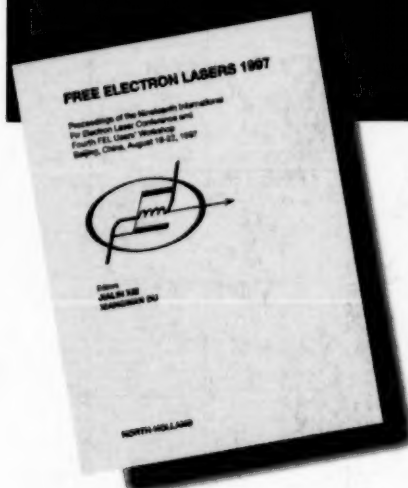
Rio de Janeiro: Elsevier Science, Rua Sete de Setembro 111/16 Andar, 20050-002 Centro, Rio de Janeiro - RJ, Brazil; phone: (+55) (21) 509 5340; fax: (+55) (21) 507 1991; e-mail: elsevier@campus.com.br [Note (Latin America): for orders, claims and help desk information, please contact the Regional Sales Office in New York as listed above]

Advertising information. Advertising orders and enquiries can be sent to: **USA, Canada and South America:** Mr Tino de Carlo, The Advertising Department, Elsevier Science Inc., 655 Avenue of the Americas, New York, NY 10010-5107, USA; phone: (+1) (212) 633 3815; fax: (+1) (212) 633 3820; e-mail: t.decarlo@elsevier.com. **Japan:** The Advertising Department, Elsevier Science K.K., 9-15 Higashi-Azabu 1-chome, Minato-ku, Tokyo 106-0044, Japan; phone: (+81) (3) 5561-5033; fax: (+81) (3) 5561 5047. **Europe and ROW:** Rachel Gresle-Farthing, The Advertising Department, Elsevier Science Ltd., The Boulevard, Langford Lane, Kidlington, Oxford OX5 1GB, UK; phone: (+44) (1865) 843565; fax: (+44) (1865) 843976; e-mail: r.gresle-farthing@elsevier.co.uk.

US mailing notice. *Chemical Physics* (ISSN 0301-0104) is published semi-monthly by Elsevier Science NL (P.O. Box 211, 1000 AE Amsterdam, The Netherlands). Annual subscription price in the USA US\$ 5125.00 (valid in North, Central and South America), including air speed delivery. Periodicals postage paid at Jamaica, NY 11431.

USA POSTMASTERS: Send address changes to: Chemical Physics, Publications Expediting Inc., 200 Meacham Avenue, Elmont, NY 11003. Airfreight and mailing in the USA by Publication Expediting Inc., 200 Meacham Avenue, Elmont, NY 11003.

Comprehensive and up-to-date coverage
of the latest research on
free electron lasers



FREE ELECTRON LASERS 1997

*Proceedings of the Nineteenth International Free
Electron Laser Conference and Fourth FEL Users'
Workshop, Beijing, China, August 18-22, 1997*

Editors

Jia-lin Xie, *IHEP, Beijing, China*
Xiang Wan Du, *IAPCM, Beijing,
China*

1998 Hardbound 702 pages
ISBN: 0-444-82978-4
Price: NLG 595.00 / US\$ 342.00



NORTH-HOLLAND
An imprint of
Elsevier Science

The last 20 years has seen
different stages of FEL
development. In this volume
the reader will find
descriptions of many new
facilities, new experimental
results, new applications,
new theoretical
developments and new
simulation results. Attention
is also focussed on the recent
progress in experimental
observations SASE.

The contributions are from
150 scientists from 13
countries, ensuring broad,
up-to-date research results
from a dynamic field.

Free Electron Lasers 1997
is a result of Part II of the
proceedings of the
conference on Free Electron
Lasers, held in Beijing,
August 1997. Part I appears
in a special issue of *Nuclear
Instruments and Methods A*.

ORDER FORM

☐ **YES!** Please send me ____ copy(ies) of
Free Electron Lasers 1997
(ISBN: 0-444-82978-4) at
NLG 595.00 / US\$ 342.00.

Name (please print) _____
Position _____
Department _____
Organisation _____
Address _____
Region/State _____
Post/Zip Code _____
Country _____
Tel _____ Fax _____
E-mail _____

NLG (Dutch Guilder) prices apply to customers in Europe and Japan.
US\$ prices apply to customers in all other countries.

PAYMENT DETAILS

- ☐ Please send a pro forma invoice.
☐ Cheque / money order / UNESCO coupon enclosed
made payable to Elsevier Science.
☐ I wish to pay by credit card (accepted from
individuals only). Your credit card will be debited
including VAT when applicable.
☐ VISA ☐ American Express ☐ MasterCard

Card No. _____

Exp. Date _____

Signature _____

Date _____

SEND YOUR ORDER TO:

For customers in the Americas:

Elsevier Science
P.O. Box 882
New York, NY 10159-0882, USA
Tel: (+1) 212-633-3730 • Fax: (+1) 212-633-3680
Toll-free for customers in the USA and Canada:
1-888-437-4636
E-mail: usinfo-f@elsevier.com

For customers in other locations:

Elsevier Science
Direct Marketing Department
P.O. Box 880
1000 AW Amsterdam
The Netherlands
Tel: (+31) 20-485-3757 • Fax: (+31) 20-485-2886
E-mail: nlinfo-f@elsevier.nl

A0339



0301-0104(199901)231/240;1-W